



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:47 AM UTC

PDB ID : 1H1Q / pdb_00001h1q
Title : Structure of human Thr160-phospho CDK2/cyclin A complexed with the inhibitor NU6094
Authors : Davies, T.G.; Noble, M.E.M.; Endicott, J.A.; Johnson, L.N.
Deposited on : 2002-07-21
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

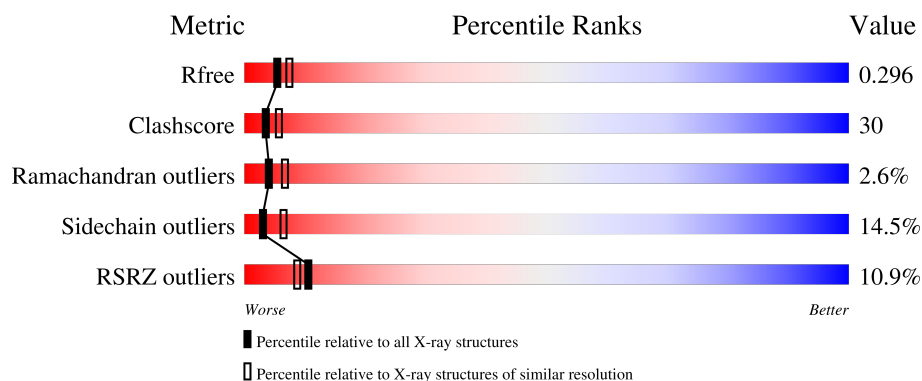
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	303	
1	C	303	
2	B	258	
2	D	258	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9325 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

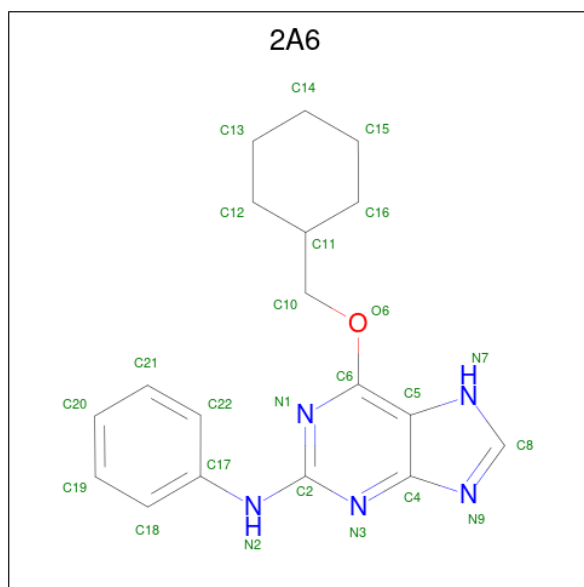
- Molecule 1 is a protein called CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	P	S	0	0	0
			2388	1550	404	425	1	8			
1	C	297	Total	C	N	O	P	S	0	0	0
			2388	1550	404	425	1	8			

- Molecule 2 is a protein called CYCLIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			
2	D	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			

- Molecule 3 is 2-ANILINO-6-CYCLOHEXYLMETHOXPURINE (CCD ID: 2A6) (formula: C₁₈H₂₁N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	18	5	1		
3	C	1	Total	C	N	O	0	0
			24	18	5	1		

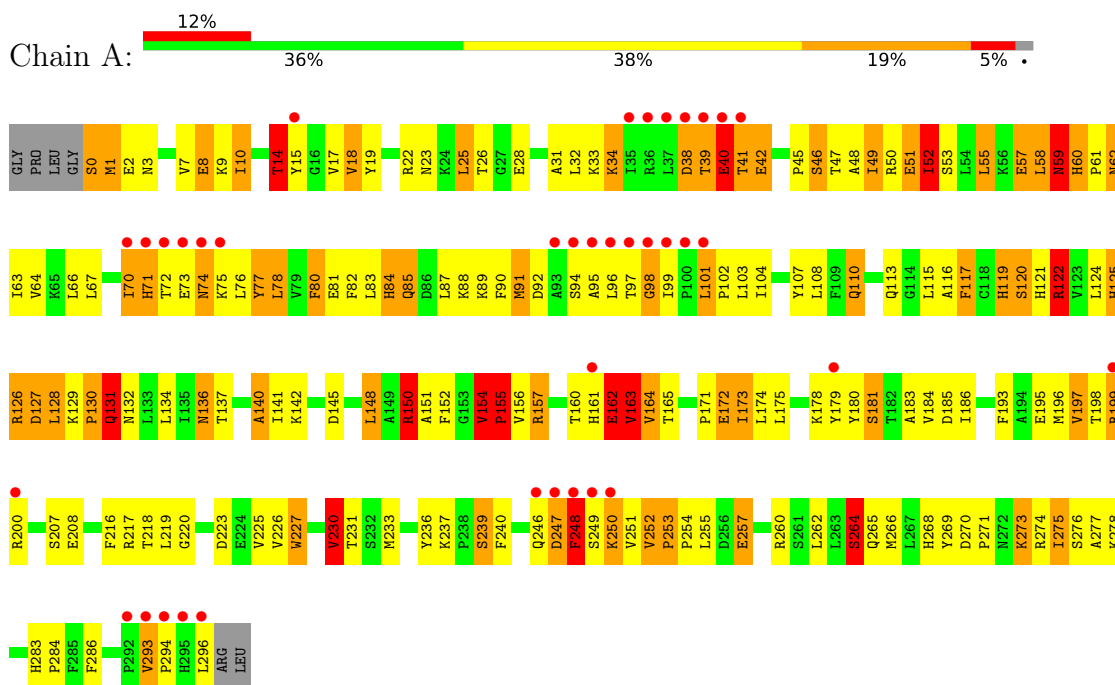
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	117	Total	O	0	0
			117	117		
4	B	87	Total	O	0	0
			87	87		
4	C	74	Total	O	0	0
			74	74		
4	D	57	Total	O	0	0
			57	57		

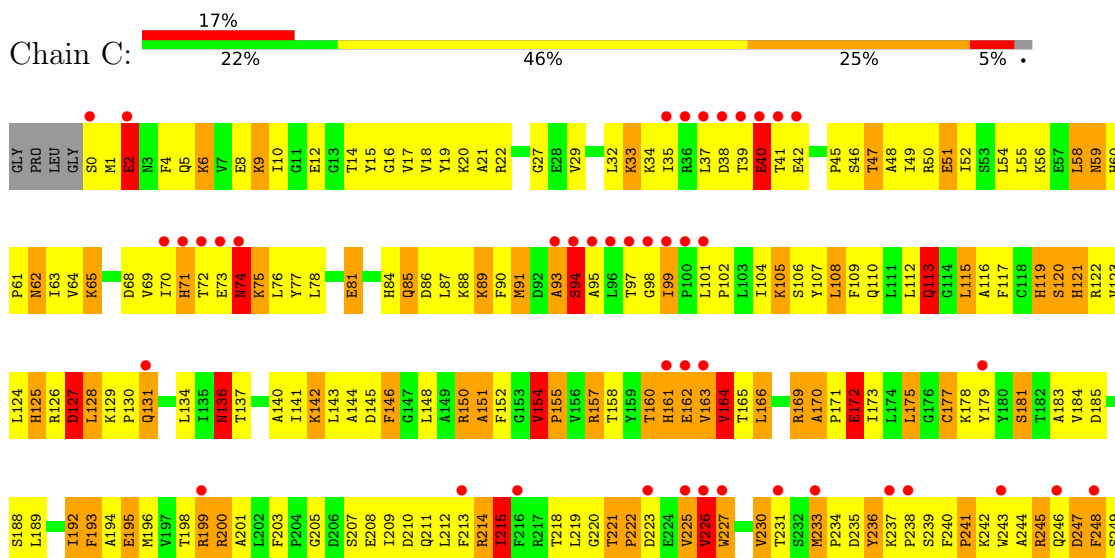
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CELL DIVISION PROTEIN KINASE 2

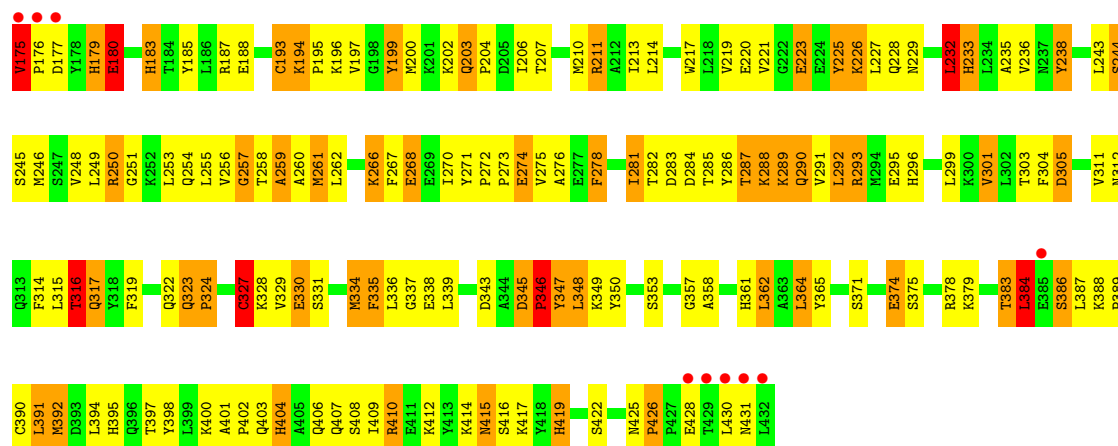


• Molecule 1: CELL DIVISION PROTEIN KINASE 2

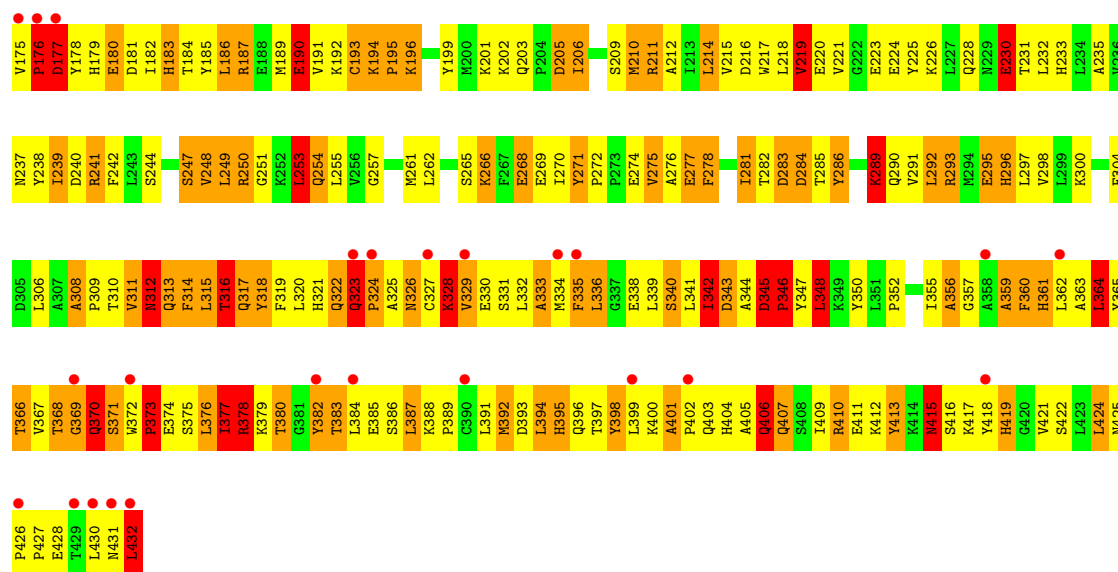
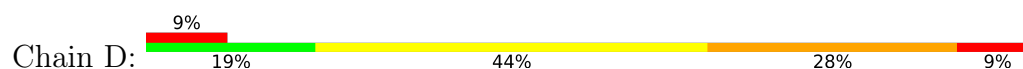




● Molecule 2: CYCLIN A2



● Molecule 2: CYCLIN A2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.99Å 134.73Å 148.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.52	Depositor EDS
% Data completeness (in resolution range)	94.1 (20.00-2.50) 94.4 (20.00-2.52)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.238 , 0.332 0.230 , 0.296	Depositor DCC
R_{free} test set	2455 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9325	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, 2A6

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.87	0/2438	2.66	177/3308 (5.4%)
1	C	0.77	0/2438	2.53	184/3308 (5.6%)
2	B	0.85	0/2133	2.60	172/2897 (5.9%)
2	D	0.79	0/2133	2.76	222/2897 (7.7%)
All	All	0.82	0/9142	2.64	755/12410 (6.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	C	0	3
2	B	0	4
2	D	0	4
All	All	0	15

There are no bond length outliers.

All (755) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	ASP	CA-CB-CG	42.58	155.18	112.60
1	A	217	ARG	CD-NE-CZ	37.79	177.31	124.40
1	C	154	VAL	CA-C-O	-26.49	101.37	119.38
2	B	345	ASP	CA-C-O	-21.62	98.11	120.38
1	C	199	ARG	CD-NE-CZ	20.95	153.73	124.40
1	C	169	ARG	CD-NE-CZ	20.31	152.84	124.40
2	D	323	GLN	CA-C-O	-19.43	102.04	119.72
1	A	154	VAL	CA-C-O	-19.17	94.26	119.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	361	HIS	CA-CB-CG	-18.39	95.41	113.80
2	B	323	GLN	CA-C-O	-15.44	104.73	119.55
1	A	80	PHE	CA-CB-CG	15.35	129.15	113.80
2	D	345	ASP	CA-C-O	-14.53	100.26	120.16
1	C	161	HIS	CA-CB-CG	-14.05	99.75	113.80
1	A	230	VAL	N-CA-CB	12.94	124.21	110.62
1	A	84	HIS	CA-CB-CG	-12.89	100.91	113.80
2	D	183	HIS	CA-CB-CG	12.87	126.67	113.80
2	B	203	GLN	CA-C-O	12.46	127.39	119.29
1	A	220	GLY	CA-C-O	-12.35	111.15	121.77
1	A	161	HIS	CA-CB-CG	-12.18	101.62	113.80
1	C	155	PRO	CA-N-CD	-11.95	95.27	112.00
2	B	283	ASP	CA-C-O	11.70	135.84	122.27
2	D	278	PHE	CA-C-O	-11.64	108.21	120.55
1	A	3	ASN	CA-C-O	-11.63	105.07	119.38
1	A	162	GLU	CB-CG-CD	11.62	132.35	112.60
1	C	193	PHE	CA-CB-CG	11.61	125.41	113.80
2	B	337	GLY	N-CA-C	-11.52	98.91	112.73
2	B	233	HIS	CA-C-O	-11.46	108.78	120.82
2	D	177	ASP	CA-CB-CG	11.29	123.89	112.60
2	B	419	HIS	CA-CB-CG	-11.22	102.58	113.80
2	D	340	SER	CA-C-O	-11.22	108.53	120.42
1	C	270	ASP	CA-C-O	11.18	128.07	119.46
2	B	179	HIS	CA-CB-CG	11.16	124.96	113.80
1	A	59	ASN	OD1-CG-ND2	10.86	133.46	122.60
2	B	324	PRO	CA-N-CD	-10.84	96.82	112.00
2	D	282	THR	CA-C-N	10.84	137.57	122.07
2	D	282	THR	C-N-CA	10.84	137.57	122.07
2	D	431	ASN	CA-CB-CG	10.81	123.41	112.60
2	B	317	GLN	OE1-CD-NE2	10.80	133.40	122.60
1	C	280	ALA	CA-C-O	-10.70	105.20	120.51
2	D	283	ASP	N-CA-CB	10.63	127.68	111.84
2	D	230	GLU	CB-CG-CD	10.57	130.58	112.60
1	A	230	VAL	CB-CA-C	-10.51	98.25	111.70
2	B	350	TYR	CA-C-O	10.50	131.84	120.71
2	D	328	LYS	N-CA-C	-10.45	100.66	113.41
2	D	194	LYS	N-CA-C	10.44	123.09	109.83
2	B	274	GLU	CB-CA-C	10.42	126.99	109.80
2	B	278	PHE	CA-CB-CG	-10.30	103.50	113.80
2	D	360	PHE	CA-CB-CG	-10.30	103.50	113.80
1	A	59	ASN	CB-CA-C	10.29	127.06	110.19
2	B	283	ASP	CA-CB-CG	10.26	122.86	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	378	ARG	CD-NE-CZ	10.22	138.70	124.40
1	C	283	HIS	CB-CA-C	10.14	122.77	108.68
1	C	214	ARG	CD-NE-CZ	10.03	138.44	124.40
2	B	193	CYS	CB-CA-C	10.01	129.13	110.11
2	D	324	PRO	CA-N-CD	-9.94	98.09	112.00
1	A	125	HIS	CA-C-O	9.87	131.19	120.24
1	A	90	PHE	CA-CB-CG	9.86	123.66	113.80
1	C	247	ASP	CA-CB-CG	9.78	122.38	112.60
1	C	230	VAL	CB-CA-C	-9.71	95.37	111.29
1	C	235	ASP	CA-CB-CG	9.60	122.20	112.60
1	C	2	GLU	CA-C-O	-9.58	110.19	120.92
2	D	395	HIS	CA-CB-CG	-9.48	104.32	113.80
1	C	260	ARG	CD-NE-CZ	9.43	137.61	124.40
1	C	85	GLN	N-CA-C	9.41	121.15	107.88
2	B	257	GLY	CA-C-O	-9.39	111.60	120.80
2	D	323	GLN	CB-CA-C	9.31	122.54	110.16
1	C	38	ASP	CA-CB-CG	9.29	121.89	112.60
1	C	125	HIS	CA-CB-CG	9.25	123.05	113.80
2	D	248	VAL	CA-C-O	-9.24	110.35	120.43
2	D	254	GLN	OE1-CD-NE2	9.24	131.84	122.60
2	D	329	VAL	N-CA-CB	9.23	122.38	110.57
2	D	355	ILE	N-CA-CB	9.23	124.42	110.58
1	C	152	PHE	CA-CB-CG	9.21	123.02	113.80
2	D	329	VAL	N-CA-C	-9.21	101.87	110.53
1	C	213	PHE	CA-C-O	-9.20	110.80	120.55
2	D	410	ARG	NE-CZ-NH2	9.18	127.46	119.20
1	A	59	ASN	CA-C-O	9.15	130.39	120.32
2	D	317	GLN	CA-C-O	9.14	130.12	120.70
2	D	322	GLN	CA-CB-CG	9.14	132.38	114.10
1	C	283	HIS	CA-CB-CG	9.14	122.94	113.80
1	C	248	PHE	CA-CB-CG	-9.08	104.72	113.80
2	B	266	LYS	CA-C-O	-9.05	110.96	120.55
1	A	40	GLU	CA-C-O	9.03	133.31	122.03
1	A	62	ASN	CA-CB-CG	-9.01	103.59	112.60
1	A	58	LEU	CA-C-N	-9.00	110.45	123.05
1	A	58	LEU	C-N-CA	-9.00	110.45	123.05
2	D	355	ILE	CA-C-O	-8.99	111.32	120.85
1	C	70	ILE	CB-CA-C	8.94	121.77	110.96
1	C	270	ASP	CB-CA-C	8.92	123.78	109.51
1	C	209	ILE	N-CA-C	-8.92	102.13	111.58
1	A	150	ARG	O-C-N	8.87	133.59	123.48
1	C	155	PRO	N-CA-CB	8.85	112.54	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	256	VAL	CA-C-N	8.83	129.92	120.03
2	B	256	VAL	C-N-CA	8.83	129.92	120.03
1	C	230	VAL	N-CA-CB	8.81	125.76	111.23
2	B	295	GLU	CA-C-O	8.80	130.24	121.00
2	D	241	ARG	NE-CZ-NH2	-8.79	111.29	119.20
2	B	187	ARG	CD-NE-CZ	8.76	136.66	124.40
1	C	184	VAL	CA-C-O	-8.76	111.94	121.05
1	A	248	PHE	CA-CB-CG	-8.71	105.08	113.80
2	D	398	TYR	CA-CB-CG	8.69	129.54	113.90
1	A	151	ALA	CA-C-O	-8.65	111.47	121.16
1	C	107	TYR	CA-CB-CG	8.64	129.46	113.90
2	D	182	ILE	CA-C-O	-8.64	111.69	120.85
2	B	323	GLN	CB-CA-C	8.61	121.67	110.13
1	C	62	ASN	CA-CB-CG	-8.61	103.99	112.60
2	D	289	LYS	CA-CB-CG	8.61	131.31	114.10
1	C	85	GLN	CB-CG-CD	-8.58	98.01	112.60
2	B	179	HIS	CA-C-O	-8.50	111.72	121.07
1	A	59	ASN	CA-CB-CG	-8.48	104.12	112.60
2	D	346	PRO	CA-N-CD	-8.44	100.19	112.00
2	D	269	GLU	N-CA-C	8.43	122.96	110.48
2	B	268	GLU	N-CA-CB	-8.42	98.16	110.53
2	D	425	ASN	CA-CB-CG	8.39	120.99	112.60
1	A	198	THR	CA-C-N	8.38	134.01	122.19
1	A	198	THR	C-N-CA	8.38	134.01	122.19
1	C	59	ASN	CB-CA-C	8.36	124.08	111.95
2	B	291	VAL	CA-C-O	8.32	129.92	121.27
1	A	246	GLN	CA-CB-CG	8.29	130.68	114.10
2	B	404	HIS	CA-CB-CG	-8.29	105.51	113.80
2	D	323	GLN	CA-CB-CG	8.27	130.65	114.10
1	A	196	MET	CA-C-N	8.27	130.81	120.72
1	A	196	MET	C-N-CA	8.27	130.81	120.72
2	B	177	ASP	N-CA-C	-8.23	102.83	113.12
1	A	252	VAL	CA-C-N	8.21	128.83	120.38
1	A	252	VAL	C-N-CA	8.21	128.83	120.38
1	A	152	PHE	CA-CB-CG	8.21	122.01	113.80
2	D	413	TYR	N-CA-C	8.19	121.66	112.97
2	D	283	ASP	CA-CB-CG	8.19	120.79	112.60
2	D	328	LYS	CA-CB-CG	8.17	130.44	114.10
2	D	378	ARG	NE-CZ-NH2	8.16	126.54	119.20
1	A	155	PRO	CA-N-CD	-8.14	100.60	112.00
1	C	192	ILE	N-CA-C	8.13	118.92	110.62
1	A	273	LYS	CA-C-O	-8.12	109.52	119.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	SER	CA-C-N	8.11	132.22	120.38
1	A	181	SER	C-N-CA	8.11	132.22	120.38
1	C	268	HIS	CA-CB-CG	-8.09	105.71	113.80
2	D	323	GLN	CA-C-N	8.06	129.91	119.84
2	D	323	GLN	C-N-CA	8.06	129.91	119.84
2	B	293	ARG	CD-NE-CZ	8.05	135.68	124.40
2	B	293	ARG	NE-CZ-NH2	8.04	126.44	119.20
1	C	272	ASN	CA-CB-CG	-8.02	104.58	112.60
1	A	216	PHE	CA-CB-CG	8.01	121.81	113.80
2	D	328	LYS	N-CA-CB	8.01	122.16	110.47
2	D	296	HIS	N-CA-CB	-7.87	98.56	110.12
2	D	403	GLN	CA-CB-CG	7.80	129.70	114.10
2	D	415	ASN	CA-CB-CG	7.78	120.38	112.60
2	B	417	LYS	CA-C-O	-7.73	112.29	120.63
2	D	428	GLU	CA-CB-CG	7.72	129.55	114.10
1	A	23	ASN	OD1-CG-ND2	-7.72	114.88	122.60
2	B	316	THR	N-CA-CB	-7.70	98.80	110.12
2	B	180	GLU	CB-CG-CD	7.68	125.66	112.60
2	D	410	ARG	CD-NE-CZ	7.68	135.16	124.40
1	A	92	ASP	CA-CB-CG	7.68	120.28	112.60
1	C	85	GLN	OE1-CD-NE2	7.67	130.27	122.60
2	D	373	PRO	CA-C-O	7.67	134.56	120.60
2	D	317	GLN	CA-C-N	7.67	136.19	121.54
2	D	317	GLN	C-N-CA	7.67	136.19	121.54
1	A	60	HIS	CA-C-O	7.66	127.19	119.76
2	B	343	ASP	CA-CB-CG	7.65	120.25	112.60
2	D	240	ASP	CA-C-O	-7.65	112.31	120.42
2	D	193	CYS	CA-C-N	7.64	131.35	120.49
2	D	193	CYS	C-N-CA	7.64	131.35	120.49
2	D	345	ASP	O-C-N	7.64	130.10	121.32
2	D	190	GLU	CA-C-O	-7.63	112.39	120.63
1	A	119	HIS	CA-C-O	7.63	128.83	120.82
2	D	214	LEU	CA-C-O	-7.62	112.81	120.82
1	C	154	VAL	CA-C-N	7.62	129.37	119.84
1	C	154	VAL	C-N-CA	7.62	129.37	119.84
2	B	392	MET	CB-CA-C	-7.62	98.62	110.81
1	A	119	HIS	CA-C-N	7.59	131.21	120.28
1	A	119	HIS	C-N-CA	7.59	131.21	120.28
2	D	364	LEU	CA-C-N	7.53	132.65	120.60
2	D	364	LEU	C-N-CA	7.53	132.65	120.60
1	A	23	ASN	CB-CG-ND2	7.53	127.69	116.40
2	B	282	THR	CA-C-N	7.53	133.51	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	282	THR	C-N-CA	7.53	133.51	122.82
2	D	295	GLU	CB-CG-CD	7.51	125.36	112.60
1	C	150	ARG	NE-CZ-NH1	-7.50	114.00	121.50
1	A	186	ILE	CA-C-N	7.49	130.32	120.28
1	A	186	ILE	C-N-CA	7.49	130.32	120.28
1	C	281	LEU	N-CA-CB	7.48	121.56	110.49
1	C	117	PHE	CA-CB-CG	-7.47	106.33	113.80
2	D	316	THR	CA-C-O	-7.44	112.59	120.63
1	A	195	GLU	CB-CG-CD	7.44	125.24	112.60
2	B	268	GLU	N-CA-C	7.41	122.61	113.50
2	B	426	PRO	O-C-N	7.40	124.71	121.31
1	A	25	LEU	N-CA-C	7.38	119.40	111.36
1	C	19	TYR	CB-CA-C	-7.37	95.36	109.66
2	D	296	HIS	CA-C-N	7.35	130.73	120.29
2	D	296	HIS	C-N-CA	7.35	130.73	120.29
2	D	177	ASP	N-CA-CB	7.34	122.89	110.49
2	B	415	ASN	CA-C-N	7.33	130.42	120.38
2	B	415	ASN	C-N-CA	7.33	130.42	120.38
1	C	275	ILE	N-CA-C	7.31	118.87	109.30
1	C	21	ALA	CA-C-N	7.30	133.08	123.00
1	C	21	ALA	C-N-CA	7.30	133.08	123.00
1	C	267	LEU	N-CA-C	7.30	122.18	113.28
1	C	195	GLU	CA-C-O	7.29	128.28	120.55
2	D	290	GLN	OE1-CD-NE2	7.29	129.89	122.60
2	B	229	ASN	CA-C-N	7.28	130.03	120.28
2	B	229	ASN	C-N-CA	7.28	130.03	120.28
2	D	312	ASN	CA-C-O	-7.27	112.84	120.55
2	D	270	ILE	CA-C-O	7.26	128.54	120.85
2	B	288	LYS	CA-C-O	7.22	128.08	120.42
1	C	214	ARG	NE-CZ-NH2	7.22	125.70	119.20
2	D	189	MET	N-CA-CB	7.21	120.47	110.01
2	B	177	ASP	CA-CB-CG	7.20	119.80	112.60
1	A	40	GLU	CA-CB-CG	7.17	128.44	114.10
1	C	62	ASN	OD1-CG-ND2	-7.15	115.45	122.60
1	C	74	ASN	CA-CB-CG	7.14	119.74	112.60
2	D	318	TYR	CA-CB-CG	7.13	126.74	113.90
1	C	58	LEU	CA-C-N	-7.13	110.44	122.92
1	C	58	LEU	C-N-CA	-7.13	110.44	122.92
1	A	122	ARG	CA-C-O	-7.13	114.00	122.27
2	B	346	PRO	CA-N-CD	-7.12	102.03	112.00
2	B	228	GLN	OE1-CD-NE2	-7.11	115.49	122.60
2	D	223	GLU	CB-CA-C	-7.11	98.76	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	PRO	N-CA-CB	7.10	110.70	103.25
2	B	414	LYS	N-CA-C	-7.09	104.44	113.23
2	D	277	GLU	CA-C-N	-7.09	110.78	120.28
2	D	277	GLU	C-N-CA	-7.09	110.78	120.28
1	A	199	ARG	CD-NE-CZ	7.08	134.32	124.40
1	A	173	ILE	N-CA-CB	7.07	119.62	110.57
2	B	415	ASN	CA-CB-CG	7.06	119.66	112.60
1	C	194	ALA	CA-C-N	7.05	129.73	120.28
1	C	194	ALA	C-N-CA	7.05	129.73	120.28
1	C	252	VAL	N-CA-CB	7.04	121.07	111.21
2	D	387	LEU	N-CA-C	7.02	121.43	113.01
2	D	219	VAL	N-CA-CB	7.02	121.11	110.58
2	D	419	HIS	CA-CB-CG	-7.01	106.79	113.80
2	B	361	HIS	CA-CB-CG	-7.00	106.80	113.80
1	C	170	ALA	N-CA-C	7.00	120.90	110.39
2	D	326	ASN	N-CA-CB	6.99	121.69	110.16
2	B	223	GLU	CB-CG-CD	-6.98	100.73	112.60
2	D	286	TYR	CA-C-N	6.96	132.64	120.87
2	D	286	TYR	C-N-CA	6.96	132.64	120.87
2	D	276	ALA	CA-C-O	-6.96	113.11	120.63
2	B	266	LYS	N-CA-CB	6.95	120.34	110.12
2	B	194	LYS	N-CA-C	6.95	118.66	109.83
2	D	321	HIS	CB-CA-C	6.95	122.66	110.85
1	C	86	ASP	CA-CB-CG	6.93	119.53	112.60
1	C	215	ILE	N-CA-CB	6.93	119.96	110.54
1	A	110	GLN	CA-C-O	-6.92	113.57	120.70
2	B	301	VAL	N-CA-C	-6.92	103.73	110.72
2	B	266	LYS	N-CA-C	-6.91	103.75	111.28
1	C	150	ARG	NE-CZ-NH2	6.89	125.41	119.20
2	D	355	ILE	CA-C-N	-6.89	110.51	120.29
2	D	355	ILE	C-N-CA	-6.89	110.51	120.29
1	A	15	TYR	CA-C-O	-6.88	113.08	121.06
2	D	220	GLU	CA-C-O	-6.87	113.55	120.90
2	D	400	LYS	CA-C-O	6.87	126.83	119.34
1	A	60	HIS	O-C-N	-6.86	116.48	121.83
1	C	18	VAL	N-CA-C	6.86	117.78	108.17
2	D	205	ASP	CA-C-O	-6.86	111.50	119.05
2	D	382	TYR	N-CA-C	-6.86	99.79	110.42
1	A	130	PRO	CA-C-N	6.86	130.15	120.28
1	A	130	PRO	C-N-CA	6.86	130.15	120.28
1	C	237	LYS	CA-CB-CG	6.86	127.81	114.10
2	D	214	LEU	N-CA-CB	6.84	119.93	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	406	GLN	CA-CB-CG	6.82	127.75	114.10
1	A	157	ARG	CB-CA-C	-6.82	98.22	110.36
2	B	180	GLU	N-CA-CB	6.82	120.14	110.12
1	A	84	HIS	CA-C-O	-6.81	113.68	120.70
1	C	274	ARG	NE-CZ-NH1	-6.81	114.69	121.50
2	B	305	ASP	CA-C-O	-6.79	114.56	122.37
2	B	285	THR	N-CA-C	-6.79	103.68	112.23
1	A	247	ASP	CA-CB-CG	6.78	119.38	112.60
2	D	355	ILE	N-CA-C	-6.77	103.89	110.72
1	A	19	TYR	CB-CA-C	-6.76	96.45	109.37
2	B	250	ARG	NE-CZ-NH1	-6.76	114.74	121.50
1	C	119	HIS	CA-C-N	6.76	129.64	120.38
1	C	119	HIS	C-N-CA	6.76	129.64	120.38
2	D	366	THR	N-CA-CB	6.74	120.65	110.14
1	C	69	VAL	CA-C-O	-6.72	111.96	120.69
2	D	241	ARG	NH1-CZ-NH2	6.71	128.03	119.30
2	D	311	VAL	N-CA-CB	-6.71	103.06	110.51
1	A	117	PHE	O-C-N	-6.71	115.01	122.12
2	B	323	GLN	O-C-N	6.69	129.33	121.10
2	B	395	HIS	CA-CB-CG	-6.69	107.11	113.80
2	B	422	SER	N-CA-C	-6.68	104.39	112.54
1	A	23	ASN	CA-CB-CG	6.65	119.25	112.60
1	A	104	ILE	CA-C-N	6.65	129.51	120.54
1	A	104	ILE	C-N-CA	6.65	129.51	120.54
1	C	172	GLU	CA-C-N	6.63	131.47	121.65
1	C	172	GLU	C-N-CA	6.63	131.47	121.65
2	D	311	VAL	CA-C-O	6.62	128.16	121.27
1	A	180	TYR	N-CA-CB	6.62	123.06	111.55
1	C	20	LYS	CA-C-O	-6.62	113.51	121.05
1	A	18	VAL	CA-C-N	6.59	132.83	122.94
1	A	18	VAL	C-N-CA	6.59	132.83	122.94
2	B	353	SER	CA-C-O	6.59	127.55	119.97
1	A	172	GLU	CB-CA-C	-6.59	99.85	110.79
2	D	176	PRO	CA-C-N	6.57	134.09	121.54
2	D	176	PRO	C-N-CA	6.57	134.09	121.54
2	B	187	ARG	NE-CZ-NH2	-6.56	113.30	119.20
1	C	58	LEU	CA-C-O	-6.55	112.89	120.49
2	B	283	ASP	N-CA-CB	6.55	121.67	111.71
2	B	232	LEU	CB-CA-C	6.53	121.14	110.88
1	A	10	ILE	CB-CA-C	-6.53	105.03	111.30
2	D	432	LEU	N-CA-CB	6.53	121.60	110.50
2	D	339	LEU	N-CA-C	-6.53	104.57	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	261	MET	CA-C-O	-6.53	112.47	119.97
1	A	131	GLN	OE1-CD-NE2	-6.51	116.08	122.60
2	D	285	THR	N-CA-C	-6.51	104.02	112.23
2	B	219	VAL	CA-C-O	6.51	128.04	121.27
1	C	59	ASN	N-CA-CB	-6.51	101.04	111.58
2	B	336	LEU	CA-C-O	6.47	127.42	120.24
2	D	253	LEU	CA-C-O	6.47	127.83	120.90
1	A	156	VAL	CA-C-N	6.47	134.63	123.05
1	A	156	VAL	C-N-CA	6.47	134.63	123.05
1	A	253	PRO	N-CA-C	6.47	118.59	110.70
1	C	93	ALA	CA-C-O	6.45	127.00	119.32
1	C	2	GLU	CB-CG-CD	6.45	123.56	112.60
1	C	245	ARG	N-CA-C	6.45	124.53	110.80
1	A	181	SER	CA-C-O	6.44	129.72	120.51
2	D	272	PRO	N-CA-C	6.44	118.55	110.70
2	B	327	CYS	CB-CA-C	6.42	123.27	110.17
2	B	199	TYR	N-CA-C	6.42	119.09	111.71
2	D	393	ASP	CA-CB-CG	-6.42	106.18	112.60
2	B	228	GLN	O-C-N	-6.41	115.25	122.75
1	A	14	THR	N-CA-CB	6.41	120.21	110.28
1	A	217	ARG	NE-CZ-NH1	-6.41	115.09	121.50
1	C	209	ILE	CB-CA-C	6.41	120.01	111.94
2	B	196	LYS	CA-CB-CG	6.39	126.89	114.10
2	B	293	ARG	NE-CZ-NH1	-6.39	115.11	121.50
2	B	290	GLN	CB-CG-CD	-6.38	101.75	112.60
1	C	166	LEU	N-CA-C	6.38	118.77	111.11
2	D	312	ASN	CB-CA-C	6.38	121.37	110.79
1	A	40	GLU	CA-C-N	6.36	133.69	121.54
1	A	40	GLU	C-N-CA	6.36	133.69	121.54
1	C	122	ARG	CA-CB-CG	6.36	126.83	114.10
2	D	277	GLU	O-C-N	6.34	128.60	122.07
1	C	113	GLN	N-CA-C	-6.33	104.30	111.14
1	C	146	PHE	CA-C-N	6.33	128.06	120.14
1	C	146	PHE	C-N-CA	6.33	128.06	120.14
2	B	343	ASP	N-CA-CB	-6.32	99.79	110.46
2	B	323	GLN	CA-C-N	6.31	127.73	119.84
2	B	323	GLN	C-N-CA	6.31	127.73	119.84
1	A	248	PHE	N-CA-C	6.31	124.24	110.80
1	C	283	HIS	CA-C-N	6.31	127.73	119.84
1	C	283	HIS	C-N-CA	6.31	127.73	119.84
2	D	318	TYR	CB-CG-CD1	6.31	130.26	120.80
2	D	270	ILE	O-C-N	-6.30	115.34	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	5	GLN	CB-CG-CD	-6.30	101.89	112.60
1	A	31	ALA	CA-C-O	-6.29	113.63	120.36
1	A	57	GLU	N-CA-C	-6.28	106.15	113.88
1	A	85	GLN	N-CA-CB	-6.28	100.72	111.21
1	C	175	LEU	CB-CA-C	6.28	122.44	109.95
2	D	345	ASP	CA-C-N	6.27	127.68	119.84
2	D	345	ASP	C-N-CA	6.27	127.68	119.84
1	C	127	ASP	CA-C-N	-6.27	110.99	121.39
1	C	127	ASP	C-N-CA	-6.27	110.99	121.39
1	C	54	LEU	CA-C-O	-6.25	114.26	120.70
1	A	71	HIS	N-CA-C	6.25	119.55	108.24
2	B	375	SER	O-C-N	-6.25	115.50	122.12
2	B	194	LYS	CB-CG-CD	6.23	125.62	111.30
2	B	220	GLU	CA-CB-CG	6.23	126.56	114.10
2	D	320	LEU	N-CA-C	-6.22	105.17	112.89
2	B	311	VAL	CA-CB-CG2	-6.22	99.82	110.40
1	C	269	TYR	CA-C-N	-6.20	112.52	121.20
1	C	269	TYR	C-N-CA	-6.20	112.52	121.20
2	D	335	PHE	CA-C-O	6.20	127.12	120.55
1	A	197	VAL	N-CA-C	6.20	116.25	110.42
2	D	360	PHE	CA-C-O	6.20	128.27	121.02
2	B	271	TYR	CA-C-O	6.19	128.03	120.54
1	A	180	TYR	CA-C-O	6.18	128.68	121.44
1	A	122	ARG	CD-NE-CZ	6.18	133.05	124.40
2	D	184	THR	CB-CA-C	6.18	120.58	110.88
1	A	70	ILE	CB-CA-C	6.17	119.08	111.25
1	A	47	THR	CA-C-N	6.16	129.04	120.29
1	A	47	THR	C-N-CA	6.16	129.04	120.29
1	A	115	LEU	CA-C-O	-6.16	113.89	120.42
1	C	145	ASP	CA-C-O	6.15	129.31	120.51
1	A	122	ARG	CG-CD-NE	6.15	125.53	112.00
2	B	243	LEU	CA-C-O	6.14	126.96	119.11
2	D	343	ASP	CA-CB-CG	-6.14	106.46	112.60
1	A	96	LEU	N-CA-C	-6.12	104.54	112.68
1	A	277	ALA	CA-C-N	6.12	128.81	120.54
1	A	277	ALA	C-N-CA	6.12	128.81	120.54
1	A	247	ASP	CA-C-N	6.11	133.21	121.54
1	A	247	ASP	C-N-CA	6.11	133.21	121.54
2	B	349	LYS	CA-CB-CG	6.10	126.30	114.10
2	D	370	GLN	CA-C-N	-6.10	112.60	122.36
2	D	370	GLN	C-N-CA	-6.10	112.60	122.36
2	B	248	VAL	N-CA-C	6.09	116.89	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	274	GLU	CA-C-N	6.09	129.12	120.53
2	B	274	GLU	C-N-CA	6.09	129.12	120.53
1	A	131	GLN	CB-CG-CD	6.09	122.95	112.60
1	A	136	ASN	CB-CG-ND2	6.09	125.53	116.40
2	D	383	THR	CB-CA-C	-6.08	99.52	112.78
2	D	319	PHE	CA-C-O	6.08	126.42	119.18
1	C	81	GLU	N-CA-C	-6.07	102.09	110.35
2	D	324	PRO	N-CD-CG	6.07	112.30	103.20
1	A	157	ARG	CA-CB-CG	6.06	126.22	114.10
2	D	314	PHE	CA-C-O	-6.05	111.85	120.51
2	B	299	LEU	CA-C-O	-6.05	113.26	120.10
1	C	68	ASP	N-CA-CB	-6.03	102.21	111.56
2	D	364	LEU	CA-C-O	6.03	129.13	120.51
2	D	321	HIS	CA-CB-CG	-6.01	107.79	113.80
2	D	317	GLN	CB-CG-CD	-6.00	102.39	112.60
2	B	274	GLU	O-C-N	-6.00	116.25	123.03
2	D	230	GLU	CA-CB-CG	6.00	126.09	114.10
2	D	342	ILE	CB-CG1-CD1	6.00	126.39	113.80
2	D	348	LEU	N-CA-C	-5.99	105.97	113.28
2	D	277	GLU	CA-C-O	-5.99	114.53	120.82
1	A	150	ARG	CA-C-O	-5.97	113.38	120.43
2	B	425	ASN	CA-CB-CG	5.97	118.57	112.60
1	C	117	PHE	CA-C-O	5.97	126.75	120.42
2	B	244	SER	CA-C-O	5.97	126.72	119.38
1	C	71	HIS	N-CA-C	5.97	119.04	108.24
1	C	268	HIS	N-CA-C	5.97	119.47	110.64
1	A	132	ASN	CA-CB-CG	-5.96	106.64	112.60
2	D	203	GLN	CA-C-O	5.96	125.18	119.99
1	C	124	LEU	N-CA-CB	5.96	120.35	110.52
1	C	121	HIS	CA-CB-CG	-5.95	107.85	113.80
2	D	398	TYR	CA-C-O	5.94	126.82	120.70
2	B	349	LYS	CB-CA-C	-5.93	99.32	109.65
2	D	254	GLN	CG-CD-OE1	-5.93	108.94	120.80
1	A	274	ARG	CD-NE-CZ	5.93	132.70	124.40
1	A	41	THR	N-CA-C	-5.92	98.18	110.80
1	A	74	ASN	CA-C-O	5.92	126.69	119.64
2	D	323	GLN	CB-CG-CD	5.92	122.66	112.60
2	D	395	HIS	N-CA-CB	-5.92	101.27	109.91
1	C	177	CYS	CA-C-O	5.91	127.66	121.15
2	B	343	ASP	O-C-N	-5.91	115.33	123.01
1	C	222	PRO	N-CA-C	-5.91	102.54	111.41
2	D	318	TYR	CB-CG-CD2	-5.91	111.93	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	268	HIS	CB-CA-C	-5.91	102.53	109.80
2	B	390	CYS	CA-C-O	5.90	126.68	120.42
2	D	278	PHE	N-CA-CB	5.90	118.80	110.12
1	A	237	LYS	CA-C-N	5.90	125.60	119.05
1	A	237	LYS	C-N-CA	5.90	125.60	119.05
2	D	304	PHE	CA-C-N	-5.90	114.10	122.41
2	D	304	PHE	C-N-CA	-5.90	114.10	122.41
2	D	359	ALA	CA-C-O	-5.90	114.30	120.55
1	C	99	ILE	CB-CA-C	-5.89	104.00	110.78
2	B	245	SER	CB-CA-C	5.88	118.18	109.29
2	B	374	GLU	CB-CG-CD	-5.88	102.61	112.60
2	D	187	ARG	N-CA-CB	5.88	118.76	110.12
1	C	50	ARG	CD-NE-CZ	-5.87	116.19	124.40
2	B	330	GLU	CB-CG-CD	5.86	122.56	112.60
1	A	246	GLN	CB-CG-CD	5.86	122.55	112.60
1	A	264	SER	O-C-N	-5.85	115.07	122.27
1	C	115	LEU	CA-C-O	5.85	126.69	119.97
1	A	140	ALA	CA-C-N	5.84	131.11	122.99
1	A	140	ALA	C-N-CA	5.84	131.11	122.99
1	C	94	SER	N-CA-C	-5.84	105.47	113.30
2	D	376	LEU	CA-CB-CG	5.84	136.73	116.30
2	D	192	LYS	CA-C-O	-5.83	114.24	120.42
2	B	383	THR	CA-CB-OG1	-5.82	100.86	109.60
2	D	211	ARG	CA-C-N	5.82	128.00	120.44
2	D	211	ARG	C-N-CA	5.82	128.00	120.44
1	A	155	PRO	N-CD-CG	5.82	111.93	103.20
2	D	407	GLN	CB-CA-C	-5.82	100.67	110.44
2	B	211	ARG	CD-NE-CZ	5.81	132.53	124.40
2	B	267	PHE	CA-CB-CG	5.80	119.60	113.80
1	C	108	LEU	N-CA-C	-5.80	104.92	112.23
1	C	238	PRO	CA-C-N	5.80	130.54	120.68
1	C	238	PRO	C-N-CA	5.80	130.54	120.68
2	D	297	LEU	N-CA-CB	5.80	118.74	110.16
1	A	58	LEU	CA-C-O	-5.79	115.40	122.41
1	C	20	LYS	CA-CB-CG	5.79	125.67	114.10
1	C	293	VAL	N-CA-CB	-5.78	104.12	111.23
1	C	29	VAL	N-CA-CB	5.78	119.11	111.25
1	C	77	TYR	CA-CB-CG	-5.78	103.50	113.90
1	C	233	MET	CA-C-N	5.76	125.89	119.32
1	C	233	MET	C-N-CA	5.76	125.89	119.32
1	A	197	VAL	CB-CA-C	-5.76	104.44	111.87
1	C	254	PRO	N-CA-C	5.76	122.33	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	113	GLN	CA-CB-CG	5.75	125.61	114.10
1	A	89	LYS	CA-C-O	-5.75	114.46	120.55
2	B	384	LEU	CA-C-O	-5.74	114.47	120.55
2	D	225	TYR	CA-C-O	5.74	126.07	119.35
2	D	377	ILE	CA-C-O	-5.74	115.08	121.05
1	C	89	LYS	CA-C-N	5.73	127.89	120.44
1	C	89	LYS	C-N-CA	5.73	127.89	120.44
2	D	217	TRP	CA-C-O	-5.73	114.80	120.82
1	C	151	ALA	N-CA-C	-5.73	102.56	110.35
2	D	241	ARG	CA-CB-CG	-5.72	102.67	114.10
2	D	308	ALA	CA-C-N	5.72	126.20	120.14
2	D	308	ALA	C-N-CA	5.72	126.20	120.14
2	D	224	GLU	CA-C-O	-5.71	114.46	120.63
2	D	325	ALA	N-CA-C	5.71	122.97	110.80
1	C	245	ARG	CA-C-O	5.70	128.66	120.51
2	B	386	SER	CA-CB-OG	5.70	122.50	111.10
1	C	127	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	163	VAL	N-CA-CB	-5.69	102.03	111.36
2	B	183	HIS	N-CA-C	-5.69	105.00	111.14
1	A	113	GLN	CA-C-O	-5.69	114.85	120.82
1	C	233	MET	N-CA-C	5.68	118.53	110.24
2	B	314	PHE	CA-C-O	-5.68	114.85	120.70
2	D	350	TYR	N-CA-C	5.68	118.81	109.72
2	D	398	TYR	N-CA-C	-5.68	105.01	111.14
1	A	46	SER	CA-CB-OG	-5.68	99.75	111.10
2	B	345	ASP	CA-C-N	5.67	126.93	119.84
2	B	345	ASP	C-N-CA	5.67	126.93	119.84
1	C	285	PHE	CA-CB-CG	5.67	119.47	113.80
1	C	84	HIS	N-CA-CB	-5.67	101.85	110.07
1	A	174	LEU	CA-C-O	-5.67	113.69	120.10
1	C	213	PHE	N-CA-CB	5.67	118.45	110.12
1	C	241	PRO	N-CA-C	-5.67	102.20	111.15
1	C	195	GLU	CA-CB-CG	5.66	125.43	114.10
2	D	210	MET	N-CA-C	-5.66	105.19	111.36
2	D	220	GLU	N-CA-CB	5.65	118.36	109.94
2	D	226	LYS	CB-CA-C	5.65	119.44	111.86
2	D	360	PHE	CB-CA-C	-5.64	101.47	110.84
2	D	379	LYS	CA-CB-CG	5.64	125.39	114.10
1	A	63	ILE	N-CA-C	-5.64	100.28	108.17
2	B	323	GLN	CB-CG-CD	5.64	122.18	112.60
2	D	293	ARG	CD-NE-CZ	5.64	132.29	124.40
2	B	175	VAL	CA-C-N	5.63	126.88	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	175	VAL	C-N-CA	5.63	126.88	119.84
1	C	128	LEU	N-CA-CB	5.63	118.85	110.29
1	C	266	MET	CA-C-O	-5.63	114.58	120.55
2	B	197	VAL	CB-CA-C	-5.62	104.56	112.14
2	D	329	VAL	CA-C-O	-5.62	114.82	121.05
2	D	230	GLU	CA-C-N	5.61	129.24	120.82
2	D	230	GLU	C-N-CA	5.61	129.24	120.82
2	D	395	HIS	CB-CA-C	5.61	119.61	110.96
2	B	235	ALA	CA-C-N	5.61	127.63	120.56
2	B	235	ALA	C-N-CA	5.61	127.63	120.56
2	D	369	GLY	N-CA-C	5.61	126.46	113.18
2	D	368	THR	CB-CA-C	-5.60	100.82	111.97
2	D	226	LYS	CB-CG-CD	5.60	124.19	111.30
2	D	251	GLY	CA-C-O	-5.60	114.35	120.40
1	C	261	SER	N-CA-C	5.60	118.92	111.75
2	B	347	TYR	O-C-N	-5.59	115.67	122.22
2	D	194	LYS	N-CA-CB	-5.59	101.18	110.02
2	D	293	ARG	NE-CZ-NH1	-5.59	115.91	121.50
1	C	29	VAL	N-CA-C	-5.59	100.34	108.17
1	A	141	ILE	O-C-N	-5.59	117.16	123.20
2	B	188	GLU	CB-CG-CD	5.59	122.11	112.60
2	D	366	THR	CB-CA-C	-5.59	100.57	111.03
1	C	95	ALA	N-CA-C	5.59	118.14	111.71
2	B	365	TYR	CA-C-N	5.58	127.75	120.28
2	B	365	TYR	C-N-CA	5.58	127.75	120.28
2	D	277	GLU	CB-CA-C	-5.58	102.13	110.88
2	D	400	LYS	CA-C-N	5.57	127.73	120.26
2	D	400	LYS	C-N-CA	5.57	127.73	120.26
2	D	290	GLN	CB-CG-CD	-5.57	103.13	112.60
2	D	360	PHE	N-CA-CB	5.57	119.18	109.72
1	A	52	ILE	CB-CA-C	-5.56	104.86	111.97
1	A	131	GLN	CG-CD-NE2	5.56	124.74	116.40
1	C	40	GLU	CA-CB-CG	5.56	125.22	114.10
2	D	314	PHE	CB-CA-C	5.55	121.47	110.42
1	A	230	VAL	CA-C-O	-5.55	115.64	121.41
1	A	273	LYS	N-CA-CB	5.55	119.17	110.46
1	C	184	VAL	N-CA-C	5.54	116.94	110.62
1	C	208	GLU	CB-CG-CD	-5.54	103.18	112.60
2	D	343	ASP	N-CA-C	5.54	118.60	107.41
2	B	225	TYR	CA-CB-CG	-5.54	103.94	113.90
1	A	171	PRO	CA-C-N	5.53	127.70	120.28
1	A	171	PRO	C-N-CA	5.53	127.70	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	256	VAL	N-CA-CB	-5.53	104.08	110.55
1	C	17	VAL	CB-CA-C	-5.53	102.38	110.62
2	B	403	GLN	CB-CA-C	-5.52	100.84	110.17
1	C	19	TYR	N-CA-C	5.51	118.56	109.85
2	D	317	GLN	O-C-N	-5.51	116.14	122.09
2	B	357	GLY	CA-C-N	5.51	127.97	120.54
2	B	357	GLY	C-N-CA	5.51	127.97	120.54
1	A	126	ARG	NE-CZ-NH1	-5.50	116.00	121.50
2	D	371	SER	CA-C-O	-5.49	115.36	121.51
1	C	283	HIS	N-CA-C	-5.49	102.74	110.31
2	D	223	GLU	CB-CG-CD	-5.49	103.28	112.60
1	A	39	THR	CB-CA-C	5.48	119.55	109.46
1	C	6	LYS	CB-CA-C	5.48	118.77	109.84
2	D	186	LEU	CA-C-O	-5.47	114.72	120.63
2	B	193	CYS	O-C-N	-5.46	114.30	122.39
2	B	387	LEU	CA-C-N	5.46	129.06	120.97
2	B	387	LEU	C-N-CA	5.46	129.06	120.97
1	C	86	ASP	CB-CA-C	5.46	118.81	109.80
1	A	257	GLU	CA-CB-CG	5.46	125.02	114.10
1	C	181	SER	CA-C-O	5.46	128.31	120.51
1	A	183	ALA	CA-C-O	-5.45	114.09	120.20
2	D	191	VAL	CB-CA-C	-5.45	104.94	112.24
1	A	217	ARG	CG-CD-NE	5.45	123.98	112.00
1	A	82	PHE	CA-C-O	-5.44	114.66	120.92
1	A	173	ILE	CA-C-O	-5.44	115.02	121.05
2	B	312	ASN	CA-C-O	-5.43	113.96	120.10
2	B	395	HIS	CA-C-O	-5.43	115.12	120.82
1	C	129	LYS	N-CA-C	-5.43	97.81	109.81
2	D	266	LYS	CG-CD-CE	5.42	123.78	111.30
2	B	317	GLN	CB-CG-CD	-5.42	103.38	112.60
1	A	51	GLU	N-CA-C	5.42	117.63	111.02
2	D	271	TYR	O-C-N	5.42	124.52	121.27
2	D	328	LYS	CB-CA-C	5.42	118.72	109.24
1	C	215	ILE	CB-CG1-CD1	5.42	125.17	113.80
2	D	268	GLU	N-CA-C	5.42	119.99	112.90
2	D	350	TYR	CA-C-O	5.42	127.23	121.11
1	A	239	SER	CA-C-O	-5.41	112.02	119.05
2	D	275	VAL	CA-C-O	-5.41	115.65	121.27
2	B	386	SER	CB-CA-C	-5.41	102.39	110.88
1	C	199	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	C	162	GLU	N-CA-C	-5.40	98.95	108.23
1	C	277	ALA	CA-C-O	5.39	126.14	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	291	VAL	N-CA-C	-5.39	105.35	110.42
1	A	247	ASP	CB-CA-C	5.39	118.35	110.26
1	C	242	LYS	CA-C-O	-5.39	114.94	120.54
1	A	208	GLU	CA-CB-CG	-5.38	103.33	114.10
1	A	227	TRP	CA-C-O	5.38	126.28	121.06
2	B	203	GLN	CB-CG-CD	5.38	121.75	112.60
1	C	119	HIS	CA-C-O	5.38	126.44	120.63
2	D	346	PRO	N-CD-CG	5.38	111.27	103.20
1	A	124	LEU	CA-C-O	-5.38	114.52	120.38
1	A	45	PRO	CB-CA-C	5.37	118.05	111.12
2	B	213	ILE	CA-C-N	5.37	127.48	120.28
2	B	213	ILE	C-N-CA	5.37	127.48	120.28
2	B	200	MET	CA-CB-CG	5.37	124.84	114.10
1	C	129	LYS	CB-CA-C	5.36	120.73	110.17
1	C	19	TYR	CA-C-O	-5.36	115.19	121.46
1	A	77	TYR	CB-CA-C	-5.35	100.46	109.72
1	A	128	LEU	CA-C-N	5.35	131.02	122.56
1	A	128	LEU	C-N-CA	5.35	131.02	122.56
2	D	209	SER	CA-C-N	-5.35	112.69	120.29
2	D	209	SER	C-N-CA	-5.35	112.69	120.29
2	B	386	SER	N-CA-CB	5.35	117.77	110.01
1	C	260	ARG	NE-CZ-NH1	5.34	126.84	121.50
2	B	335	PHE	O-C-N	-5.34	116.46	122.12
2	D	324	PRO	N-CA-CB	5.34	108.86	103.25
2	D	333	ALA	CA-C-O	5.34	126.40	120.90
1	A	122	ARG	NE-CZ-NH1	5.33	126.83	121.50
1	C	51	GLU	CA-CB-CG	-5.33	103.45	114.10
1	A	199	ARG	CG-CD-NE	5.32	123.71	112.00
1	A	218	THR	CB-CA-C	-5.32	101.86	110.79
1	C	185	ASP	N-CA-CB	5.32	118.52	110.28
1	A	1	MET	CA-C-N	5.32	129.64	121.19
1	A	1	MET	C-N-CA	5.32	129.64	121.19
1	C	91	MET	CA-CB-CG	5.32	124.73	114.10
2	B	343	ASP	N-CA-C	5.31	118.09	107.62
1	C	169	ARG	NE-CZ-NH1	5.31	126.81	121.50
2	D	401	ALA	N-CA-C	-5.31	105.52	112.75
1	C	247	ASP	CB-CA-C	5.31	117.81	110.16
1	A	165	THR	O-C-N	-5.30	116.34	122.87
2	B	283	ASP	CA-C-N	5.30	131.66	121.54
2	B	283	ASP	C-N-CA	5.30	131.66	121.54
1	A	117	PHE	CA-C-N	5.29	127.63	120.44
1	A	117	PHE	C-N-CA	5.29	127.63	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	281	ILE	CA-C-O	-5.28	114.18	120.78
2	B	378	ARG	CA-C-O	-5.28	114.95	120.55
2	D	182	ILE	CB-CA-C	5.28	119.50	112.22
1	A	246	GLN	CB-CA-C	5.27	119.16	109.46
2	B	397	THR	CA-CB-OG1	-5.27	101.69	109.60
1	C	150	ARG	N-CA-C	5.27	118.02	108.69
1	C	276	SER	CA-CB-OG	5.26	121.63	111.10
1	C	274	ARG	CD-NE-CZ	-5.26	117.03	124.40
1	A	184	VAL	N-CA-CB	5.26	118.47	110.58
1	A	134	LEU	O-C-N	-5.26	117.06	123.16
2	D	195	PRO	CB-CA-C	-5.26	102.55	110.17
2	D	322	GLN	N-CA-CB	5.26	117.77	109.83
2	B	281	ILE	N-CA-CB	5.25	119.90	111.23
1	A	198	THR	CA-C-O	5.25	125.83	119.11
1	C	253	PRO	CA-C-N	5.25	125.30	119.32
1	C	253	PRO	C-N-CA	5.25	125.30	119.32
1	A	67	LEU	CA-C-O	-5.24	113.94	119.97
1	A	157	ARG	NE-CZ-NH2	-5.24	114.48	119.20
2	B	422	SER	N-CA-CB	5.24	119.09	110.39
2	B	213	ILE	CA-C-O	-5.24	115.62	121.17
2	B	259	ALA	CA-C-O	5.23	126.09	120.70
1	C	162	GLU	CB-CA-C	5.23	119.89	111.05
1	A	250	LYS	CB-CA-C	5.22	120.15	109.55
1	C	41	THR	N-CA-C	-5.22	99.69	110.80
2	D	297	LEU	CA-C-O	-5.21	114.90	120.42
2	B	311	VAL	CA-C-O	5.21	126.37	120.95
1	C	162	GLU	N-CA-CB	-5.20	102.69	110.24
1	A	172	GLU	CA-CB-CG	5.20	124.50	114.10
2	B	343	ASP	CA-C-N	5.20	127.97	120.38
2	B	343	ASP	C-N-CA	5.20	127.97	120.38
1	A	252	VAL	CA-C-O	5.19	126.91	119.95
1	A	85	GLN	CA-CB-CG	5.19	124.48	114.10
2	B	251	GLY	N-CA-C	-5.19	107.48	115.73
2	B	238	TYR	CB-CA-C	-5.18	102.19	110.79
1	C	22	ARG	CB-CA-C	-5.18	100.76	109.72
2	D	223	GLU	O-C-N	5.18	128.06	122.15
2	B	245	SER	O-C-N	-5.18	116.44	121.93
2	B	254	GLN	CA-C-N	5.18	127.17	120.44
2	B	254	GLN	C-N-CA	5.18	127.17	120.44
1	C	37	LEU	N-CA-C	-5.17	103.57	110.55
1	C	237	LYS	CA-C-N	5.17	124.78	119.56
1	C	237	LYS	C-N-CA	5.17	124.78	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	371	SER	N-CA-C	5.17	117.72	109.81
1	C	136	ASN	N-CA-CB	5.17	118.40	110.49
2	B	258	THR	O-C-N	-5.17	116.26	122.15
1	C	227	TRP	CA-CB-CG	5.17	123.41	113.60
2	B	314	PHE	N-CA-C	-5.16	105.56	111.14
1	A	22	ARG	CA-CB-CG	5.16	124.42	114.10
1	C	209	ILE	CA-C-O	-5.16	114.73	120.46
2	D	255	LEU	CA-C-O	-5.16	115.08	120.55
1	C	235	ASP	N-CA-C	-5.16	104.17	110.61
2	B	407	GLN	CA-CB-CG	5.15	124.41	114.10
2	D	398	TYR	CB-CG-CD1	5.15	128.53	120.80
1	A	85	GLN	CB-CG-CD	-5.15	103.84	112.60
2	D	342	ILE	CB-CA-C	-5.15	103.92	112.26
2	B	315	LEU	CA-C-N	5.15	127.18	120.28
2	B	315	LEU	C-N-CA	5.15	127.18	120.28
2	D	340	SER	O-C-N	-5.15	116.28	122.15
1	C	157	ARG	N-CA-C	-5.15	101.54	109.52
2	B	410	ARG	CB-CG-CD	5.14	123.12	111.30
2	D	356	ALA	N-CA-C	-5.14	105.76	111.36
2	B	197	VAL	N-CA-CB	5.13	117.52	110.54
2	B	378	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	A	286	PHE	N-CA-C	5.13	119.17	113.02
2	D	278	PHE	N-CA-C	-5.13	105.69	111.28
2	D	336	LEU	CA-C-O	-5.13	115.42	120.70
1	C	65	LYS	N-CA-C	5.12	117.11	108.96
1	C	255	LEU	CA-CB-CG	5.12	134.23	116.30
1	A	49	ILE	CA-C-O	-5.12	115.62	120.95
2	D	340	SER	CB-CA-C	5.12	119.56	110.85
1	A	132	ASN	CA-C-N	-5.12	115.84	123.11
1	A	132	ASN	C-N-CA	-5.12	115.84	123.11
2	B	259	ALA	O-C-N	-5.11	116.57	122.09
2	B	414	LYS	CA-C-O	-5.11	113.30	119.27
1	C	162	GLU	CB-CG-CD	5.11	121.28	112.60
1	C	5	GLN	N-CA-CB	5.10	118.56	110.55
1	C	142	LYS	CA-C-N	5.10	128.58	121.24
1	C	142	LYS	C-N-CA	5.10	128.58	121.24
2	D	405	ALA	N-CA-C	5.09	118.96	112.34
2	D	394	LEU	N-CA-C	5.09	116.83	111.28
1	C	77	TYR	CB-CA-C	-5.09	100.22	109.38
1	C	290	THR	N-CA-CB	5.09	119.09	110.49
1	C	4	PHE	CA-CB-CG	-5.08	108.72	113.80
1	A	14	THR	CA-CB-CG2	5.08	119.14	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	180	GLU	CA-CB-CG	5.08	124.27	114.10
2	D	262	LEU	CA-C-O	5.08	126.16	120.82
2	D	379	LYS	O-C-N	5.08	128.01	122.11
2	B	287	THR	N-CA-CB	5.08	117.70	110.44
2	B	180	GLU	CA-CB-CG	5.08	124.26	114.10
2	D	271	TYR	CB-CA-C	-5.08	104.99	110.98
2	D	378	ARG	NE-CZ-NH1	-5.07	116.43	121.50
1	C	237	LYS	CA-C-O	5.07	124.86	119.69
2	D	209	SER	CA-C-O	-5.07	113.67	119.60
2	D	410	ARG	NE-CZ-NH1	-5.06	116.44	121.50
1	A	132	ASN	CA-C-O	-5.05	113.16	119.28
2	B	374	GLU	CB-CA-C	5.05	119.18	110.79
2	B	426	PRO	CA-C-O	-5.05	117.26	120.90
2	D	368	THR	N-CA-C	5.04	117.27	110.06
1	A	165	THR	CA-CB-CG2	5.04	119.07	110.50
2	D	371	SER	N-CA-C	5.04	116.65	109.14
2	B	276	ALA	CA-C-O	5.04	126.29	120.90
1	A	26	THR	CA-CB-CG2	5.04	119.06	110.50
2	D	221	VAL	CB-CA-C	-5.04	105.44	112.04
2	D	249	LEU	CA-C-O	5.04	127.75	121.81
1	A	293	VAL	N-CA-CB	-5.03	105.37	111.31
2	B	407	GLN	CB-CA-C	-5.02	102.00	110.44
1	A	275	ILE	O-C-N	-5.02	117.14	122.61
2	D	193	CYS	CB-CA-C	5.02	119.65	110.36
2	D	380	THR	CA-C-O	-5.01	115.11	120.42
2	B	334	MET	CA-C-N	5.01	126.99	120.28
2	B	334	MET	C-N-CA	5.01	126.99	120.28
1	A	196	MET	CB-CA-C	5.01	119.10	110.79
1	C	177	CYS	CB-CA-C	5.01	117.76	109.70
1	C	236	TYR	CA-CB-CG	-5.01	104.89	113.90
1	A	217	ARG	N-CA-C	-5.01	106.01	111.82
1	C	152	PHE	CB-CA-C	5.01	120.05	109.79
2	B	324	PRO	N-CA-CB	5.00	108.50	103.25

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	0	SER	Mainchain
1	A	122	ARG	Mainchain
1	A	154	VAL	Mainchain,Peptide
2	B	323	GLN	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
2	B	345	ASP	Mainchain,Peptide
1	C	0	SER	Mainchain
1	C	154	VAL	Mainchain,Peptide
2	D	323	GLN	Mainchain,Peptide
2	D	345	ASP	Mainchain,Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2388	0	2430	127	0
1	C	2388	0	2429	193	0
2	B	2083	0	2107	86	0
2	D	2083	0	2107	168	0
3	A	24	0	21	2	0
3	C	24	0	21	2	0
4	A	117	0	0	13	0
4	B	87	0	0	7	0
4	C	74	0	0	13	0
4	D	57	0	0	12	0
All	All	9325	0	9115	538	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (538) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:210:MET:HE1	2:D:250:ARG:HB2	1.28	1.10
2:D:367:VAL:HG12	2:D:368:THR:HG23	1.43	0.99
1:A:84:HIS:HD2	1:A:136:ASN:HA	1.31	0.95
2:D:378:ARG:HB2	2:D:378:ARG:HH21	1.33	0.91
1:C:64:VAL:HG21	1:C:144:ALA:HB2	1.52	0.90
1:A:14:THR:HG21	1:A:148:LEU:HD22	1.54	0.88
1:C:60:HIS:HD2	1:C:62:ASN:H	1.21	0.86
2:D:315:LEU:HG	2:D:356:ALA:HB1	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ALA:O	1:C:120:SER:HB2	1.76	0.84
1:C:262:LEU:HG	1:C:266:MET:HE2	1.61	0.83
1:C:115:LEU:HD22	1:C:189:LEU:HD12	1.62	0.82
1:C:223:ASP:H	1:C:226:VAL:HG13	1.44	0.81
2:D:315:LEU:HG	2:D:356:ALA:CB	2.10	0.81
1:A:39:THR:HB	2:B:289:LYS:HE3	1.62	0.80
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.62	0.79
1:A:60:HIS:HD2	1:A:62:ASN:H	1.30	0.78
2:B:210:MET:HE1	2:B:250:ARG:HB2	1.64	0.78
1:C:113:GLN:HB3	4:C:2023:HOH:O	1.85	0.77
2:D:377:ILE:HG13	2:D:382:TYR:O	1.84	0.77
1:A:181:SER:HB3	4:A:2073:HOH:O	1.85	0.76
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.51	0.75
1:C:88:LYS:HD2	1:C:131:GLN:HE21	1.51	0.75
2:D:233:HIS:CE1	4:D:2036:HOH:O	2.39	0.74
1:A:60:HIS:CD2	1:A:62:ASN:H	2.05	0.73
2:D:424:LEU:H	2:D:424:LEU:HD23	1.52	0.73
2:D:216:ASP:OD2	2:D:406:GLN:HB3	1.89	0.72
2:D:183:HIS:HB2	2:D:317:GLN:NE2	2.05	0.71
1:A:84:HIS:CD2	1:A:136:ASN:HA	2.22	0.71
2:D:401:ALA:N	2:D:402:PRO:HD2	2.07	0.69
2:D:206:ILE:HG21	2:D:253:LEU:HD22	1.74	0.69
1:C:128:LEU:HD12	1:C:189:LEU:HG	1.73	0.69
1:C:45:PRO:HB2	1:C:47:THR:HG23	1.75	0.68
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.74	0.68
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.75	0.68
2:B:207:THR:OG1	2:B:210:MET:HG3	1.94	0.68
1:C:71:HIS:CD2	1:C:76:LEU:HD13	2.29	0.68
1:C:170:ALA:HB1	1:C:172:GLU:OE2	1.94	0.67
1:C:280:ALA:O	1:C:286:PHE:HE2	1.77	0.67
1:A:25:LEU:HD11	2:D:293:ARG:HB3	1.76	0.67
2:B:175:VAL:N	2:B:176:PRO:HD3	2.09	0.67
1:A:10:ILE:HD12	1:A:18:VAL:HG12	1.75	0.67
1:C:231:THR:HG22	1:C:236:TYR:CZ	2.29	0.67
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.76	0.67
1:C:203:PHE:HB3	4:C:2058:HOH:O	1.95	0.67
1:C:214:ARG:HB2	4:C:2058:HOH:O	1.95	0.67
1:C:246:GLN:HG2	1:C:251:VAL:HG23	1.76	0.67
1:A:88:LYS:HB2	1:A:130:PRO:HB2	1.78	0.66
2:B:388:LYS:HG3	2:B:392:MET:HE3	1.78	0.66
2:B:273:PRO:HB2	2:B:278:PHE:CE2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:364:LEU:HD21	2:D:370:GLN:CD	2.19	0.66
1:A:53:SER:HB3	2:B:304:PHE:O	1.96	0.66
1:A:137:THR:HG22	1:A:296:LEU:HD12	1.76	0.66
1:C:60:HIS:CD2	1:C:62:ASN:H	2.11	0.66
2:D:326:ASN:HD21	2:D:328:LYS:HD3	1.61	0.66
1:A:51:GLU:O	1:A:55:LEU:HB2	1.96	0.66
1:C:154:VAL:O	2:D:316:THR:HG23	1.95	0.66
1:A:155:PRO:HD2	2:B:316:THR:HG23	1.78	0.65
1:C:33:LYS:HD2	1:C:78:LEU:HD12	1.79	0.65
2:D:368:THR:O	2:D:370:GLN:HG3	1.97	0.65
1:C:126:ARG:NH2	1:C:160:TPO:O3P	2.29	0.65
2:D:327:CYS:HB3	4:D:2034:HOH:O	1.97	0.65
2:D:375:SER:HA	2:D:378:ARG:CZ	2.27	0.65
1:C:223:ASP:H	1:C:226:VAL:CG1	2.10	0.64
1:A:108:LEU:HD21	1:A:266:MET:HE1	1.80	0.64
2:B:262:LEU:HD11	2:B:266:LYS:HE3	1.79	0.64
2:D:377:ILE:HD11	2:D:383:THR:HG22	1.78	0.64
2:D:218:LEU:HD22	2:D:261:MET:SD	2.38	0.64
2:D:314:PHE:O	2:D:315:LEU:C	2.40	0.64
1:A:219:LEU:HD23	4:A:2085:HOH:O	1.98	0.64
2:D:230:GLU:OE1	2:D:312:ASN:ND2	2.32	0.63
2:D:347:TYR:OH	2:D:394:LEU:HA	1.99	0.63
1:C:178:LYS:HG2	4:C:2048:HOH:O	1.97	0.63
2:B:327:CYS:HB2	4:B:2057:HOH:O	1.98	0.63
1:C:58:LEU:HB3	1:C:63:ILE:HD12	1.80	0.62
2:D:210:MET:HE1	2:D:250:ARG:CB	2.18	0.62
1:C:49:ILE:HG23	2:D:306:LEU:HD12	1.82	0.62
2:D:344:ALA:HA	2:D:348:LEU:HD22	1.81	0.62
1:C:195:GLU:HG2	1:C:201:ALA:HA	1.80	0.62
1:A:18:VAL:HA	1:A:32:LEU:O	1.99	0.62
1:C:136:ASN:HD21	1:C:140:ALA:HB3	1.64	0.62
1:C:273:LYS:O	1:C:274:ARG:C	2.42	0.62
1:C:287:GLN:HG2	1:C:288:ASP:N	2.13	0.62
2:D:378:ARG:HB2	2:D:378:ARG:NH2	2.11	0.62
1:C:227:TRP:O	1:C:230:VAL:HG23	2.00	0.62
1:C:241:PRO:HG2	1:C:243:TRP:CH2	2.34	0.62
2:D:187:ARG:NH2	2:D:382:TYR:OH	2.32	0.62
1:C:261:SER:O	1:C:265:GLN:HG3	2.00	0.61
2:D:395:HIS:CG	2:D:430:LEU:HD11	2.34	0.61
1:C:88:LYS:HD2	1:C:131:GLN:NE2	2.13	0.61
1:A:116:ALA:O	1:A:120:SER:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:211:ARG:O	2:D:215:VAL:HG23	2.01	0.61
1:A:9:LYS:NZ	1:A:17:VAL:HG11	2.15	0.61
1:A:33:LYS:HD2	1:A:80:PHE:HE1	1.66	0.61
2:B:176:PRO:HA	2:B:179:HIS:CG	2.36	0.61
2:B:176:PRO:HA	2:B:179:HIS:ND1	2.16	0.61
2:D:289:LYS:HE2	2:D:293:ARG:NH2	2.16	0.61
1:A:154:VAL:HG13	2:B:179:HIS:CE1	2.36	0.61
2:D:266:LYS:NZ	2:D:295:GLU:OE2	2.34	0.60
2:D:233:HIS:HE1	4:D:2036:HOH:O	1.78	0.60
2:D:426:PRO:HG3	4:D:2048:HOH:O	2.00	0.60
2:D:364:LEU:HD22	2:D:370:GLN:HB2	1.84	0.59
2:B:358:ALA:HA	2:B:391:LEU:HD22	1.83	0.59
1:C:160:TPO:HG23	1:C:162:GLU:O	2.01	0.59
1:A:39:THR:HB	2:B:289:LYS:CE	2.30	0.59
1:A:137:THR:HG22	1:A:296:LEU:CD1	2.32	0.59
2:D:406:GLN:HB2	4:D:2050:HOH:O	2.03	0.59
1:A:75:LYS:HB2	4:A:2031:HOH:O	2.02	0.59
1:C:40:GLU:HA	2:D:292:LEU:HD23	1.84	0.59
2:D:235:ALA:O	2:D:239:ILE:HG13	2.02	0.59
2:D:315:LEU:CG	2:D:356:ALA:HB1	2.30	0.59
2:B:194:LYS:HG3	2:B:195:PRO:HD2	1.85	0.59
2:D:364:LEU:CD2	2:D:370:GLN:HB2	2.33	0.59
1:C:15:TYR:CE1	1:C:33:LYS:HE2	2.38	0.58
2:D:404:HIS:HB3	4:D:2049:HOH:O	2.04	0.58
1:A:7:VAL:O	1:A:8:GLU:HB3	2.03	0.58
2:D:411:GLU:O	2:D:412:LYS:C	2.44	0.58
2:D:342:ILE:HD11	2:D:409:ILE:HD12	1.83	0.58
1:A:253:PRO:HB2	1:A:254:PRO:HD3	1.86	0.58
2:B:194:LYS:HG3	2:B:195:PRO:CD	2.34	0.58
2:B:287:THR:N	2:B:290:GLN:OE1	2.30	0.58
2:D:374:GLU:O	2:D:377:ILE:HG22	2.04	0.58
2:B:233:HIS:HD2	4:B:2050:HOH:O	1.87	0.58
2:D:313:GLN:O	2:D:316:THR:HG22	2.04	0.58
1:C:240:PHE:O	1:C:241:PRO:C	2.47	0.58
1:A:154:VAL:HB	2:B:317:GLN:HG3	1.86	0.57
1:C:125:HIS:CE1	1:C:128:LEU:HD23	2.38	0.57
1:A:1:MET:SD	1:A:70:ILE:HD13	2.44	0.57
1:A:163:VAL:HG12	1:A:173:ILE:HD13	1.85	0.57
1:C:87:LEU:O	1:C:91:MET:HG2	2.03	0.57
1:C:112:LEU:HB2	1:C:281:LEU:CD2	2.34	0.57
1:A:40:GLU:HB3	2:B:288:LYS:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:ALA:HB1	1:C:274:ARG:NH1	2.20	0.57
2:D:205:ASP:OD2	2:D:250:ARG:HB3	2.04	0.57
1:A:72:THR:HA	4:A:2029:HOH:O	2.04	0.57
1:C:272:ASN:ND2	1:C:272:ASN:H	2.01	0.57
1:C:210:ASP:O	1:C:214:ARG:HG3	2.03	0.57
1:C:72:THR:HB	1:C:75:LYS:O	2.03	0.57
1:C:231:THR:HA	1:C:236:TYR:CD1	2.40	0.57
1:C:137:THR:HG23	4:C:2038:HOH:O	2.03	0.57
1:C:219:LEU:HB3	1:C:269:TYR:HE2	1.70	0.57
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.40	0.56
2:D:336:LEU:HD13	2:D:362:LEU:HD23	1.87	0.56
2:D:401:ALA:O	2:D:402:PRO:C	2.48	0.56
1:A:17:VAL:HB	4:A:2011:HOH:O	2.03	0.56
1:C:42:GLU:OE1	2:D:275:VAL:HG23	2.06	0.56
2:D:364:LEU:HD21	2:D:370:GLN:NE2	2.20	0.56
1:A:58:LEU:HA	1:A:117:PHE:HE2	1.71	0.56
1:C:188:SER:O	1:C:192:ILE:HG13	2.05	0.56
2:D:315:LEU:HD22	2:D:333:ALA:HB1	1.86	0.56
1:A:64:VAL:HG11	3:A:1298:2A6:H8	1.88	0.56
2:B:388:LYS:O	2:B:392:MET:HG2	2.05	0.56
1:A:172:GLU:HG3	1:A:271:PRO:HG3	1.88	0.56
2:D:421:VAL:HA	2:D:424:LEU:HD21	1.88	0.56
1:C:90:PHE:O	1:C:94:SER:HB2	2.06	0.56
2:D:175:VAL:N	2:D:176:PRO:HD3	2.22	0.55
1:C:115:LEU:HG	1:C:119:HIS:CD2	2.42	0.55
2:D:233:HIS:CE1	2:D:341:LEU:HD11	2.41	0.55
1:C:115:LEU:CD2	1:C:189:LEU:HD12	2.35	0.55
2:D:329:VAL:HG21	2:D:364:LEU:HA	1.89	0.55
2:D:331:SER:OG	2:D:418:TYR:HA	2.05	0.55
1:A:162:GLU:CD	1:A:162:GLU:H	2.15	0.55
1:A:223:ASP:H	1:A:226:VAL:CG1	2.19	0.55
1:C:64:VAL:CG2	1:C:144:ALA:HB2	2.30	0.55
2:D:404:HIS:O	2:D:407:GLN:NE2	2.40	0.55
1:C:104:ILE:O	1:C:108:LEU:N	2.37	0.54
1:C:115:LEU:HD22	1:C:189:LEU:CD1	2.33	0.54
1:C:198:THR:HG22	1:C:252:VAL:HG13	1.88	0.54
1:A:83:LEU:HD23	1:A:136:ASN:HB3	1.90	0.54
2:D:346:PRO:HD2	2:D:347:TYR:CE2	2.42	0.54
2:D:371:SER:O	2:D:372:TRP:C	2.50	0.54
2:D:395:HIS:ND1	2:D:430:LEU:HD21	2.22	0.54
1:C:85:GLN:O	1:C:134:LEU:HA	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:360:PHE:CD2	2:D:376:LEU:HD11	2.43	0.54
2:D:424:LEU:HD23	2:D:424:LEU:N	2.21	0.54
1:C:46:SER:HB3	2:D:266:LYS:HB3	1.89	0.54
1:C:131:GLN:CD	1:C:131:GLN:H	2.14	0.54
1:A:172:GLU:CG	1:A:271:PRO:HG3	2.38	0.54
1:C:62:ASN:HA	1:C:142:LYS:HG2	1.88	0.54
2:B:362:LEU:HD13	2:B:430:LEU:HD21	1.89	0.54
2:B:404:HIS:CE1	2:B:406:GLN:HB2	2.43	0.54
1:C:64:VAL:HG23	1:C:143:LEU:O	2.07	0.54
2:D:187:ARG:HD3	4:D:2003:HOH:O	2.08	0.54
2:D:426:PRO:HB2	2:D:427:PRO:HD2	1.89	0.54
1:C:112:LEU:HB2	1:C:281:LEU:HD21	1.90	0.54
1:A:84:HIS:HD2	1:A:136:ASN:CA	2.14	0.53
2:B:401:ALA:HB1	2:B:410:ARG:HD2	1.90	0.53
2:D:242:PHE:CD1	2:D:298:VAL:HG22	2.42	0.53
2:D:328:LYS:HB2	2:D:421:VAL:HG12	1.89	0.53
1:A:9:LYS:HZ2	1:A:17:VAL:HG11	1.73	0.53
1:C:210:ASP:CG	1:C:214:ARG:HD2	2.34	0.53
1:A:0:SER:C	1:A:2:GLU:H	2.16	0.53
1:A:98:GLY:HA3	1:A:199:ARG:NH1	2.24	0.53
1:C:255:LEU:HG	1:C:259:GLY:HA3	1.89	0.53
1:C:51:GLU:HG3	1:C:146:PHE:HB2	1.89	0.53
1:C:115:LEU:HG	1:C:119:HIS:NE2	2.24	0.53
1:C:253:PRO:HD2	1:C:254:PRO:HD2	1.91	0.53
1:A:40:GLU:H	2:B:292:LEU:HD23	1.74	0.53
2:B:305:ASP:HA	4:B:2047:HOH:O	2.08	0.53
2:D:233:HIS:HB3	2:D:310:THR:HG21	1.91	0.53
2:B:180:GLU:OE1	2:B:379:LYS:NZ	2.40	0.53
2:D:237:ASN:O	2:D:238:TYR:C	2.52	0.53
2:D:289:LYS:HE2	2:D:293:ARG:HH22	1.74	0.53
1:A:33:LYS:HD2	1:A:80:PHE:CE1	2.44	0.52
2:D:274:GLU:H	2:D:277:GLU:HG3	1.74	0.52
1:A:260:ARG:O	1:A:264:SER:HB3	2.09	0.52
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.74	0.52
2:B:303:THR:O	2:B:304:PHE:HB2	2.09	0.52
2:B:347:TYR:OH	2:B:394:LEU:HA	2.09	0.52
1:C:40:GLU:HA	2:D:292:LEU:CD2	2.40	0.52
1:C:200:ARG:NH1	1:C:200:ARG:HG3	2.23	0.52
1:C:231:THR:HA	1:C:236:TYR:CG	2.44	0.52
2:D:296:HIS:NE2	2:D:300:LYS:NZ	2.54	0.52
2:D:395:HIS:NE2	2:D:399:LEU:HD11	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:419:HIS:HB3	4:B:2082:HOH:O	2.09	0.52
2:D:342:ILE:HD11	2:D:409:ILE:CD1	2.40	0.52
2:D:415:ASN:OD1	2:D:416:SER:N	2.42	0.52
1:C:136:ASN:ND2	1:C:140:ALA:HB3	2.24	0.52
2:D:332:LEU:O	2:D:336:LEU:HG	2.10	0.51
1:C:250:LYS:O	1:C:251:VAL:C	2.52	0.51
2:D:194:LYS:NZ	2:D:195:PRO:HD2	2.25	0.51
2:D:328:LYS:HB2	2:D:421:VAL:CG1	2.40	0.51
1:C:108:LEU:HD22	1:C:193:PHE:CG	2.46	0.51
1:A:95:ALA:HA	1:A:199:ARG:HD2	1.93	0.51
2:D:331:SER:HB3	2:D:421:VAL:HG21	1.92	0.51
2:B:262:LEU:O	2:B:266:LYS:HG3	2.10	0.51
1:C:42:GLU:OE1	2:D:274:GLU:HB2	2.11	0.51
1:C:175:LEU:HG	1:C:212:LEU:HD21	1.93	0.51
1:C:227:TRP:CD2	1:C:230:VAL:HG22	2.46	0.51
1:C:249:SER:O	1:C:253:PRO:HA	2.10	0.51
1:A:227:TRP:HB3	1:A:230:VAL:HG22	1.92	0.51
1:C:74:ASN:HB2	1:C:75:LYS:HD2	1.92	0.51
1:C:137:THR:HA	1:C:296:LEU:CD1	2.41	0.51
1:C:6:LYS:HE3	1:C:32:LEU:CD1	2.41	0.51
1:C:154:VAL:HB	2:D:317:GLN:HG3	1.92	0.51
1:C:215:ILE:HD13	4:C:2058:HOH:O	2.10	0.51
2:D:315:LEU:HG	2:D:356:ALA:HB2	1.90	0.51
1:C:109:PHE:CE1	1:C:281:LEU:HB3	2.46	0.51
2:D:335:PHE:CD2	2:D:336:LEU:HD23	2.46	0.51
2:D:372:TRP:HB3	2:D:384:LEU:HD11	1.92	0.51
1:A:101:LEU:HB3	1:A:102:PRO:HD3	1.93	0.51
1:C:161:HIS:HB3	1:C:162:GLU:OE2	2.11	0.51
2:D:317:GLN:HA	4:D:2032:HOH:O	2.10	0.51
2:D:365:TYR:HB2	2:D:370:GLN:O	2.11	0.51
1:A:230:VAL:HA	1:A:233:MET:SD	2.51	0.50
1:C:259:GLY:O	1:C:260:ARG:C	2.52	0.50
2:D:335:PHE:HB2	2:D:413:TYR:CD2	2.46	0.50
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.46	0.50
1:C:109:PHE:HE1	1:C:281:LEU:HB3	1.75	0.50
2:B:232:LEU:O	2:B:236:VAL:HG23	2.11	0.50
2:D:230:GLU:O	2:D:233:HIS:HB2	2.11	0.50
1:A:95:ALA:HA	1:A:199:ARG:CD	2.42	0.50
2:D:175:VAL:HG22	2:D:177:ASP:OD2	2.12	0.50
1:A:178:LYS:HG3	1:A:179:TYR:CE2	2.46	0.50
1:C:15:TYR:CE2	1:C:48:ALA:HB2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:ARG:HG3	1:C:200:ARG:HH11	1.76	0.50
2:D:187:ARG:NH2	2:D:382:TYR:CZ	2.80	0.50
2:D:368:THR:O	2:D:370:GLN:N	2.41	0.50
1:A:98:GLY:HA2	1:A:199:ARG:HD3	1.94	0.49
1:A:131:GLN:CD	1:A:131:GLN:H	2.19	0.49
2:D:361:HIS:ND1	2:D:372:TRP:N	2.60	0.49
1:A:129:LYS:HG3	1:A:131:GLN:HG2	1.94	0.49
1:C:225:VAL:O	1:C:226:VAL:C	2.55	0.49
2:B:289:LYS:CE	2:B:289:LYS:HA	2.41	0.49
1:C:52:ILE:O	1:C:56:LYS:HG3	2.12	0.49
1:C:65:LYS:HB3	1:C:81:GLU:HG2	1.93	0.49
1:C:227:TRP:CZ3	1:C:269:TYR:HD1	2.31	0.49
1:C:253:PRO:CB	1:C:254:PRO:HD3	2.37	0.49
2:D:340:SER:O	2:D:341:LEU:C	2.55	0.49
2:B:214:LEU:HD22	2:B:253:LEU:HG	1.95	0.49
1:C:72:THR:HG22	1:C:73:GLU:H	1.77	0.49
2:B:211:ARG:HG2	2:B:211:ARG:HH11	1.77	0.49
1:C:198:THR:CG2	1:C:252:VAL:HG13	2.42	0.49
1:C:256:ASP:OD2	1:C:259:GLY:N	2.39	0.49
1:C:278:LYS:HB2	2:D:178:TYR:CE1	2.48	0.49
1:C:121:HIS:HD2	2:D:185:TYR:CE1	2.31	0.48
1:C:220:GLY:O	1:C:221:THR:C	2.56	0.48
2:D:407:GLN:OE1	2:D:410:ARG:HG3	2.12	0.48
1:A:178:LYS:HG3	1:A:179:TYR:CD2	2.48	0.48
1:A:262:LEU:HG	1:A:266:MET:HE2	1.94	0.48
2:B:327:CYS:SG	2:B:419:HIS:NE2	2.86	0.48
2:D:418:TYR:O	2:D:419:HIS:HB2	2.13	0.48
1:A:1:MET:SD	1:A:70:ILE:HG21	2.53	0.48
1:A:99:ILE:HG23	1:A:103:LEU:HD23	1.95	0.48
2:B:194:LYS:NZ	2:B:195:PRO:O	2.46	0.48
1:C:278:LYS:NZ	2:D:181:ASP:OD2	2.47	0.48
1:C:227:TRP:CE3	1:C:269:TYR:HD1	2.32	0.48
1:C:253:PRO:HB2	1:C:254:PRO:CD	2.39	0.48
2:D:421:VAL:O	2:D:424:LEU:HG	2.13	0.48
1:A:57:GLU:OE1	2:B:185:TYR:OH	2.29	0.48
1:C:286:PHE:O	1:C:287:GLN:C	2.57	0.48
2:D:193:CYS:O	2:D:241:ARG:HD2	2.13	0.48
1:A:34:LYS:HB3	4:A:2011:HOH:O	2.13	0.48
1:A:40:GLU:CB	2:B:288:LYS:HD3	2.44	0.48
1:A:268:HIS:CD2	1:A:273:LYS:HB2	2.47	0.48
1:C:101:LEU:N	1:C:102:PRO:HD2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:370:GLN:HB2	4:D:2040:HOH:O	2.12	0.48
1:C:33:LYS:HD3	1:C:35:ILE:HD11	1.96	0.48
1:C:137:THR:HA	1:C:296:LEU:HD12	1.94	0.48
2:B:400:LYS:O	2:B:401:ALA:C	2.56	0.48
2:D:196:LYS:HG2	2:D:199:TYR:HB3	1.95	0.48
2:D:210:MET:CE	2:D:250:ARG:HD3	2.43	0.48
2:D:401:ALA:N	2:D:402:PRO:CD	2.74	0.48
1:A:94:SER:O	1:A:98:GLY:N	2.47	0.47
2:B:289:LYS:HA	2:B:289:LYS:HE2	1.95	0.47
1:C:106:SER:O	1:C:110:GLN:HG3	2.14	0.47
3:C:1298:2A6:C22	3:C:1298:2A6:N1	2.76	0.47
2:D:254:GLN:HG2	2:D:286:TYR:HE2	1.78	0.47
1:C:262:LEU:O	1:C:265:GLN:N	2.47	0.47
1:A:14:THR:HG23	1:A:145:ASP:OD1	2.15	0.47
1:C:58:LEU:HD21	1:C:123:VAL:HG21	1.96	0.47
2:D:375:SER:HA	2:D:378:ARG:NH2	2.29	0.47
1:C:40:GLU:HG3	2:D:289:LYS:HZ1	1.80	0.47
1:C:172:GLU:CD	1:C:274:ARG:HH22	2.22	0.47
1:C:268:HIS:O	1:C:269:TYR:C	2.58	0.47
2:D:277:GLU:O	2:D:278:PHE:C	2.57	0.47
2:D:329:VAL:HG13	2:D:363:ALA:CB	2.45	0.47
2:D:364:LEU:HD23	2:D:364:LEU:C	2.40	0.47
1:C:15:TYR:CZ	1:C:33:LYS:HE2	2.49	0.47
1:C:171:PRO:HD2	1:C:172:GLU:OE2	2.14	0.47
1:C:178:LYS:HE2	1:C:179:TYR:CE2	2.49	0.47
1:C:193:PHE:CZ	1:C:255:LEU:HD11	2.49	0.47
1:C:223:ASP:O	1:C:226:VAL:HG13	2.14	0.47
2:D:230:GLU:HG3	2:D:268:GLU:CD	2.39	0.47
1:A:125:HIS:ND1	1:A:128:LEU:HD23	2.29	0.47
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.96	0.47
1:A:59:ASN:HA	4:A:2024:HOH:O	2.14	0.47
1:A:197:VAL:HG11	1:A:252:VAL:CG1	2.44	0.47
2:B:404:HIS:ND1	2:B:406:GLN:HB2	2.30	0.47
1:C:193:PHE:CE1	1:C:255:LEU:HD11	2.49	0.47
1:A:163:VAL:HG13	1:A:164:VAL:HG23	1.95	0.46
2:B:322:GLN:NE2	2:B:330:GLU:OE2	2.47	0.46
2:D:338:GLU:HG2	2:D:409:ILE:HD13	1.96	0.46
1:A:231:THR:HG22	1:A:236:TYR:CZ	2.50	0.46
2:D:239:ILE:CD1	2:D:257:GLY:HA2	2.46	0.46
2:D:315:LEU:CD2	2:D:356:ALA:HB1	2.45	0.46
2:D:375:SER:HA	2:D:378:ARG:NH1	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ILE:HD11	1:A:78:LEU:CD2	2.45	0.46
2:B:259:ALA:O	2:B:260:ALA:C	2.55	0.46
2:B:329:VAL:HG11	2:B:364:LEU:HD12	1.98	0.46
1:C:88:LYS:O	1:C:89:LYS:C	2.58	0.46
1:C:157:ARG:HD3	2:D:228:GLN:OE1	2.16	0.46
1:C:231:THR:HG22	1:C:236:TYR:CE2	2.51	0.46
1:A:154:VAL:O	2:B:316:THR:CG2	2.63	0.46
2:B:384:LEU:HD12	2:B:384:LEU:HA	1.90	0.46
1:C:207:SER:H	1:C:210:ASP:HB3	1.79	0.46
2:D:329:VAL:CG2	2:D:364:LEU:HA	2.45	0.46
1:A:119:HIS:HE1	1:A:185:ASP:OD2	1.99	0.46
1:A:178:LYS:HG2	4:A:2071:HOH:O	2.15	0.46
1:C:219:LEU:HD13	4:C:2070:HOH:O	2.16	0.46
2:B:175:VAL:N	2:B:176:PRO:CD	2.79	0.46
2:B:335:PHE:CZ	2:B:339:LEU:HD11	2.51	0.46
1:C:225:VAL:O	1:C:227:TRP:N	2.49	0.46
2:D:343:ASP:O	2:D:344:ALA:C	2.58	0.46
2:D:409:ILE:O	2:D:410:ARG:C	2.58	0.46
1:A:251:VAL:HG12	1:A:252:VAL:HG23	1.98	0.46
1:A:48:ALA:O	1:A:52:ILE:HG13	2.16	0.46
1:A:223:ASP:H	1:A:226:VAL:HG12	1.81	0.46
1:A:249:SER:O	1:A:253:PRO:HA	2.16	0.46
1:A:262:LEU:CG	1:A:266:MET:HE2	2.45	0.46
1:A:270:ASP:HB3	1:A:273:LYS:HG2	1.97	0.46
1:C:244:ALA:HB2	4:C:2066:HOH:O	2.16	0.46
1:A:62:ASN:HA	1:A:142:LYS:HG2	1.96	0.46
1:A:253:PRO:CB	1:A:254:PRO:HD3	2.46	0.46
2:B:223:GLU:CD	2:B:412:LYS:HG3	2.41	0.45
2:B:288:LYS:O	2:B:292:LEU:HB2	2.16	0.45
1:C:163:VAL:HG12	1:C:164:VAL:HG23	1.98	0.45
1:C:272:ASN:HB3	4:C:2072:HOH:O	2.16	0.45
1:A:265:GLN:HB3	1:A:275:ILE:HB	1.98	0.45
1:C:99:ILE:HD13	1:C:196:MET:HG2	1.97	0.45
2:D:359:ALA:O	2:D:360:PHE:C	2.58	0.45
2:B:330:GLU:O	2:B:334:MET:HG3	2.16	0.45
1:C:6:LYS:HE3	1:C:32:LEU:HD13	1.99	0.45
2:B:398:TYR:CD2	2:B:426:PRO:HB3	2.51	0.45
1:C:169:ARG:HD3	1:C:173:ILE:HG21	1.98	0.45
3:C:1298:2A6:N1	3:C:1298:2A6:H22	2.31	0.45
2:D:388:LYS:HD2	2:D:432:LEU:HD13	1.98	0.45
2:B:316:THR:HG21	4:B:2053:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:SER:O	1:C:98:GLY:N	2.49	0.45
1:C:172:GLU:OE1	1:C:274:ARG:NH1	2.30	0.45
1:C:258:ASP:OD2	1:C:284:PRO:HB2	2.15	0.45
1:A:175:LEU:HB2	1:A:233:MET:HE2	1.98	0.45
1:C:87:LEU:HB3	1:C:130:PRO:CB	2.46	0.45
1:C:137:THR:O	1:C:293:VAL:HG13	2.16	0.45
2:D:214:LEU:O	2:D:214:LEU:HD12	2.17	0.45
2:D:383:THR:N	2:D:386:SER:OG	2.49	0.45
2:D:360:PHE:HD2	2:D:376:LEU:HD11	1.81	0.45
1:C:284:PRO:O	1:C:285:PHE:C	2.60	0.45
2:B:415:ASN:OD1	2:B:416:SER:N	2.50	0.45
1:C:205:GLY:HA2	1:C:210:ASP:OD2	2.17	0.45
1:C:51:GLU:O	1:C:55:LEU:HB2	2.17	0.45
1:C:1:MET:O	1:C:2:GLU:C	2.60	0.44
1:C:257:GLU:HA	1:C:260:ARG:NH2	2.33	0.44
1:C:262:LEU:O	1:C:263:LEU:C	2.59	0.44
2:D:216:ASP:HA	2:D:219:VAL:HG23	1.98	0.44
2:D:248:VAL:HG12	2:D:249:LEU:O	2.17	0.44
2:D:335:PHE:HD2	2:D:336:LEU:HD23	1.82	0.44
1:C:178:LYS:HG3	1:C:179:TYR:CD2	2.52	0.44
2:D:308:ALA:HA	2:D:309:PRO:HD3	1.83	0.44
2:D:387:LEU:O	2:D:391:LEU:HB2	2.17	0.44
1:C:279:ALA:O	1:C:281:LEU:N	2.50	0.44
2:D:391:LEU:HD12	4:D:2044:HOH:O	2.17	0.44
2:D:418:TYR:O	2:D:421:VAL:HG13	2.18	0.44
1:A:51:GLU:HG3	1:A:55:LEU:HD22	2.00	0.44
1:A:71:HIS:NE2	2:B:296:HIS:CE1	2.85	0.44
1:A:81:GLU:HB2	4:A:2034:HOH:O	2.17	0.44
2:B:217:TRP:O	2:B:221:VAL:HG23	2.17	0.44
2:B:249:LEU:HG	1:C:27:GLY:HA3	1.99	0.44
2:B:338:GLU:HG2	2:B:409:ILE:HD13	1.98	0.44
1:C:93:ALA:HB3	4:C:2034:HOH:O	2.17	0.44
2:D:315:LEU:O	2:D:318:TYR:HB2	2.18	0.44
1:C:222:PRO:HD3	1:C:269:TYR:CE1	2.52	0.44
2:D:356:ALA:O	2:D:357:GLY:C	2.60	0.44
1:A:103:LEU:HD11	1:A:107:TYR:CZ	2.52	0.44
1:C:63:ILE:O	1:C:64:VAL:C	2.58	0.44
1:C:101:LEU:N	1:C:102:PRO:CD	2.80	0.44
1:C:171:PRO:O	1:C:172:GLU:C	2.61	0.44
2:D:332:LEU:HD21	2:D:398:TYR:OH	2.18	0.44
2:B:227:LEU:HD12	2:B:261:MET:HE2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:ARG:O	1:C:127:ASP:HB2	2.17	0.44
2:D:338:GLU:HG2	2:D:409:ILE:CD1	2.47	0.44
2:B:255:LEU:HB2	2:B:286:TYR:CZ	2.53	0.43
1:C:279:ALA:O	1:C:280:ALA:C	2.59	0.43
1:A:72:THR:HG22	1:A:73:GLU:H	1.83	0.43
1:A:207:SER:HB3	4:A:2080:HOH:O	2.17	0.43
1:A:283:HIS:CE1	1:A:284:PRO:HG2	2.52	0.43
1:C:192:ILE:HG22	1:C:196:MET:CE	2.48	0.43
2:D:212:ALA:HA	2:D:342:ILE:HG22	2.00	0.43
1:A:130:PRO:HD2	1:A:131:GLN:OE1	2.18	0.43
1:C:128:LEU:HD22	1:C:143:LEU:HD22	1.99	0.43
1:C:263:LEU:HD11	1:C:267:LEU:HD11	1.98	0.43
2:D:190:GLU:HG3	2:D:352:PRO:HD2	2.00	0.43
1:A:283:HIS:CG	1:A:284:PRO:HD2	2.53	0.43
2:B:199:TYR:CE2	2:B:348:LEU:HD21	2.53	0.43
1:C:48:ALA:O	1:C:49:ILE:C	2.60	0.43
1:C:163:VAL:O	1:C:164:VAL:O	2.37	0.43
1:A:39:THR:CB	2:B:289:LYS:HZ2	2.31	0.43
2:B:319:PHE:O	2:B:322:GLN:HG3	2.18	0.43
1:C:212:LEU:O	1:C:215:ILE:HG12	2.19	0.43
1:A:154:VAL:HB	2:B:317:GLN:CG	2.49	0.43
2:B:401:ALA:HB3	2:B:402:PRO:HD3	2.01	0.43
1:C:210:ASP:OD1	1:C:214:ARG:HD2	2.19	0.43
1:A:157:ARG:NH2	2:B:268:GLU:OE2	2.45	0.43
2:D:345:ASP:OD1	2:D:345:ASP:C	2.62	0.43
1:C:74:ASN:HA	4:C:2033:HOH:O	2.18	0.43
1:C:233:MET:HA	1:C:234:PRO:HD3	1.88	0.43
1:A:28:GLU:HG3	2:D:247:SER:HB3	2.01	0.43
1:A:57:GLU:CD	2:B:185:TYR:HH	2.27	0.43
1:C:162:GLU:H	1:C:162:GLU:CD	2.26	0.43
1:A:110:GLN:OE1	1:A:140:ALA:HA	2.19	0.43
1:A:193:PHE:O	1:A:197:VAL:HG23	2.19	0.43
1:A:293:VAL:HA	1:A:294:PRO:HD2	1.88	0.43
2:B:225:TYR:O	2:B:226:LYS:HB2	2.19	0.43
1:A:101:LEU:N	1:A:102:PRO:CD	2.82	0.42
1:A:239:SER:O	1:A:240:PHE:C	2.60	0.42
1:C:222:PRO:HD3	1:C:269:TYR:CZ	2.53	0.42
2:B:238:TYR:N	2:B:238:TYR:CD1	2.87	0.42
2:B:270:ILE:HG13	4:B:2040:HOH:O	2.19	0.42
1:C:189:LEU:HD23	1:C:189:LEU:HA	1.80	0.42
1:A:150:ARG:HG2	4:A:2050:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:331:SER:HA	2:D:334:MET:HG3	2.00	0.42
1:A:50:ARG:HD3	4:A:2049:HOH:O	2.19	0.42
1:A:236:TYR:CD1	1:A:236:TYR:C	2.97	0.42
1:C:236:TYR:CD1	1:C:236:TYR:C	2.96	0.42
1:A:126:ARG:O	1:A:127:ASP:HB2	2.19	0.42
1:C:60:HIS:HB3	1:C:63:ILE:HG13	2.02	0.42
1:C:105:LYS:NZ	1:C:285:PHE:O	2.51	0.42
1:C:158:THR:HA	1:C:178:LYS:O	2.20	0.42
2:D:230:GLU:O	2:D:233:HIS:N	2.53	0.42
2:D:347:TYR:CD2	2:D:347:TYR:N	2.86	0.42
1:A:98:GLY:HA3	1:A:199:ARG:HH11	1.84	0.42
1:A:101:LEU:CB	1:A:102:PRO:HD3	2.50	0.42
1:C:171:PRO:O	1:C:173:ILE:N	2.53	0.42
1:C:280:ALA:O	1:C:286:PHE:CE2	2.66	0.42
1:C:283:HIS:HA	1:C:284:PRO:HD2	1.72	0.42
2:D:283:ASP:O	2:D:284:ASP:C	2.63	0.42
2:D:371:SER:O	2:D:373:PRO:N	2.53	0.42
1:A:87:LEU:O	1:A:91:MET:HB2	2.19	0.42
1:C:233:MET:HB2	1:C:236:TYR:HB2	2.02	0.42
2:B:430:LEU:O	2:B:431:ASN:HB2	2.20	0.42
1:A:269:TYR:O	1:A:271:PRO:HD3	2.20	0.41
1:C:268:HIS:HD2	1:C:270:ASP:H	1.67	0.41
2:D:254:GLN:HB3	2:D:286:TYR:OH	2.20	0.41
1:A:53:SER:HB2	4:B:2048:HOH:O	2.20	0.41
1:C:42:GLU:CD	2:D:275:VAL:HG23	2.45	0.41
1:C:253:PRO:CB	1:C:254:PRO:CD	2.97	0.41
2:D:185:TYR:O	2:D:186:LEU:C	2.61	0.41
2:D:194:LYS:HZ2	2:D:195:PRO:HD2	1.84	0.41
2:B:203:GLN:HA	2:B:204:PRO:HD2	1.92	0.41
2:D:178:TYR:O	2:D:179:HIS:C	2.61	0.41
2:D:327:CYS:HA	2:D:330:GLU:HB2	2.01	0.41
1:A:52:ILE:HG12	1:A:78:LEU:CD1	2.51	0.41
1:A:52:ILE:HG12	1:A:78:LEU:HD11	2.03	0.41
1:C:269:TYR:O	1:C:274:ARG:NH2	2.49	0.41
2:D:383:THR:H	2:D:386:SER:CB	2.33	0.41
2:B:211:ARG:HG2	2:B:211:ARG:NH1	2.35	0.41
1:C:9:LYS:HG2	1:C:10:ILE:N	2.34	0.41
2:B:246:MET:HG3	2:B:301:VAL:HG21	2.01	0.41
2:D:392:MET:HE1	2:D:430:LEU:CD1	2.50	0.41
1:A:101:LEU:N	1:A:102:PRO:HD2	2.36	0.41
1:A:121:HIS:HD2	2:B:185:TYR:CE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:SER:O	1:C:240:PHE:C	2.64	0.41
1:C:273:LYS:HA	1:C:273:LYS:HD3	1.90	0.41
1:A:40:GLU:HA	2:B:288:LYS:CE	2.50	0.41
1:A:98:GLY:CA	1:A:199:ARG:NH1	2.84	0.41
1:C:150:ARG:HG2	1:C:151:ALA:O	2.21	0.41
1:C:162:GLU:O	1:C:163:VAL:HG23	2.20	0.41
1:C:210:ASP:OD2	1:C:214:ARG:HD2	2.21	0.41
1:C:227:TRP:CG	1:C:230:VAL:HG22	2.55	0.41
2:D:210:MET:HE1	2:D:250:ARG:HD3	2.01	0.41
2:D:228:GLN:O	2:D:231:THR:HB	2.21	0.41
1:C:166:LEU:HD11	1:C:211:GLN:HB2	2.03	0.41
1:C:173:ILE:HG21	4:C:2042:HOH:O	2.21	0.41
2:D:219:VAL:HG21	2:D:409:ILE:HG13	2.02	0.41
1:A:219:LEU:HA	4:A:2085:HOH:O	2.21	0.40
1:A:223:ASP:OD1	1:A:225:VAL:N	2.54	0.40
2:B:214:LEU:HD11	2:B:257:GLY:HA3	2.02	0.40
2:D:366:THR:HG23	4:D:2056:HOH:O	2.20	0.40
1:A:1:MET:HE2	1:A:77:TYR:CG	2.55	0.40
1:C:49:ILE:CG2	2:D:306:LEU:HD12	2.50	0.40
1:C:164:VAL:O	1:C:165:THR:C	2.62	0.40
1:C:171:PRO:HD3	4:C:2046:HOH:O	2.21	0.40
2:D:175:VAL:N	2:D:176:PRO:CD	2.83	0.40
2:D:329:VAL:HA	2:D:367:VAL:HG21	2.03	0.40
2:B:255:LEU:HD12	2:B:255:LEU:HA	1.88	0.40
1:C:134:LEU:O	1:C:141:ILE:HA	2.21	0.40
1:C:275:ILE:HG23	1:C:275:ILE:O	2.20	0.40
2:D:219:VAL:HG11	2:D:409:ILE:HG12	2.04	0.40
2:D:335:PHE:CE1	2:D:422:SER:HB3	2.56	0.40
1:A:42:GLU:OE1	2:B:275:VAL:HG23	2.21	0.40
1:A:72:THR:O	2:B:296:HIS:HE1	2.05	0.40
1:A:85:GLN:HA	3:A:1298:2A6:C20	2.52	0.40
1:A:136:ASN:ND2	1:A:140:ALA:HB3	2.35	0.40
2:B:272:PRO:HA	2:B:273:PRO:HD3	1.94	0.40
2:B:327:CYS:SG	2:B:419:HIS:CE1	3.14	0.40
1:C:274:ARG:HH11	1:C:274:ARG:HD2	1.39	0.40
2:D:241:ARG:O	2:D:244:SER:HB2	2.21	0.40
2:D:314:PHE:O	2:D:317:GLN:N	2.52	0.40
2:D:397:THR:HG23	4:D:2047:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	294/303 (97%)	274 (93%)	11 (4%)	9 (3%)	3	5
1	C	294/303 (97%)	251 (85%)	33 (11%)	10 (3%)	3	4
2	B	256/258 (99%)	244 (95%)	9 (4%)	3 (1%)	10	20
2	D	256/258 (99%)	219 (86%)	30 (12%)	7 (3%)	4	6
All	All	1100/1122 (98%)	988 (90%)	83 (8%)	29 (3%)	4	7

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	164	VAL
1	C	225	VAL
2	D	346	PRO
2	D	369	GLY
1	A	38	ASP
1	A	98	GLY
1	A	127	ASP
1	A	164	VAL
1	A	248	PHE
2	B	346	PRO
1	C	172	GLU
1	C	226	VAL
1	C	280	ALA
1	A	8	GLU
1	A	162	GLU
1	C	127	ASP
1	C	245	ARG
2	D	177	ASP
2	B	324	PRO
1	C	155	PRO
1	C	274	ARG
2	D	315	LEU

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Mol	Chain	Res	Type
1	A	41	THR
2	D	176	PRO
1	A	155	PRO
2	B	281	ILE
1	C	16	GLY
2	D	281	ILE
2	D	373	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/265 (98%)	228 (87%)	33 (13%)	4	9
1	C	261/265 (98%)	223 (85%)	38 (15%)	3	6
2	B	232/232 (100%)	204 (88%)	28 (12%)	5	10
2	D	232/232 (100%)	188 (81%)	44 (19%)	1	3
All	All	986/994 (99%)	843 (86%)	143 (14%)	3	6

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	34	LYS
1	A	40	GLU
1	A	42	GLU
1	A	46	SER
1	A	49	ILE
1	A	52	ILE
1	A	55	LEU
1	A	59	ASN
1	A	66	LEU
1	A	74	ASN
1	A	76	LEU
1	A	78	LEU
1	A	91	MET

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Mol	Chain	Res	Type
1	A	97	THR
1	A	101	LEU
1	A	120	SER
1	A	122	ARG
1	A	131	GLN
1	A	148	LEU
1	A	150	ARG
1	A	162	GLU
1	A	163	VAL
1	A	200	ARG
1	A	230	VAL
1	A	247	ASP
1	A	248	PHE
1	A	250	LYS
1	A	255	LEU
1	A	257	GLU
1	A	264	SER
1	A	276	SER
1	A	278	LYS
2	B	175	VAL
2	B	180	GLU
2	B	193	CYS
2	B	202	LYS
2	B	206	ILE
2	B	226	LYS
2	B	232	LEU
2	B	244	SER
2	B	274	GLU
2	B	284	ASP
2	B	289	LYS
2	B	292	LEU
2	B	293	ARG
2	B	316	THR
2	B	327	CYS
2	B	328	LYS
2	B	331	SER
2	B	346	PRO
2	B	348	LEU
2	B	362	LEU
2	B	364	LEU
2	B	374	GLU
2	B	383	THR

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Mol	Chain	Res	Type
2	B	384	LEU
2	B	386	SER
2	B	391	LEU
2	B	408	SER
2	B	428	GLU
1	C	2	GLU
1	C	8	GLU
1	C	9	LYS
1	C	12	GLU
1	C	14	THR
1	C	33	LYS
1	C	34	LYS
1	C	39	THR
1	C	40	GLU
1	C	47	THR
1	C	59	ASN
1	C	74	ASN
1	C	75	LYS
1	C	94	SER
1	C	97	THR
1	C	105	LYS
1	C	113	GLN
1	C	120	SER
1	C	131	GLN
1	C	136	ASN
1	C	148	LEU
1	C	163	VAL
1	C	164	VAL
1	C	177	CYS
1	C	181	SER
1	C	199	ARG
1	C	200	ARG
1	C	215	ILE
1	C	218	THR
1	C	221	THR
1	C	226	VAL
1	C	247	ASP
1	C	248	PHE
1	C	252	VAL
1	C	281	LEU
1	C	287	GLN
1	C	289	VAL

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Mol	Chain	Res	Type
1	C	290	THR
2	D	177	ASP
2	D	180	GLU
2	D	190	GLU
2	D	196	LYS
2	D	201	LYS
2	D	202	LYS
2	D	206	ILE
2	D	219	VAL
2	D	230	GLU
2	D	232	LEU
2	D	239	ILE
2	D	247	SER
2	D	250	ARG
2	D	253	LEU
2	D	265	SER
2	D	271	TYR
2	D	281	ILE
2	D	284	ASP
2	D	289	LYS
2	D	292	LEU
2	D	311	VAL
2	D	312	ASN
2	D	313	GLN
2	D	316	THR
2	D	322	GLN
2	D	323	GLN
2	D	324	PRO
2	D	328	LYS
2	D	342	ILE
2	D	346	PRO
2	D	348	LEU
2	D	364	LEU
2	D	370	GLN
2	D	377	ILE
2	D	378	ARG
2	D	380	THR
2	D	385	GLU
2	D	392	MET
2	D	396	GLN
2	D	406	GLN
2	D	415	ASN

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Mol	Chain	Res	Type
2	D	417	LYS
2	D	424	LEU
2	D	432	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	74	ASN
1	A	84	HIS
1	A	119	HIS
1	A	265	GLN
2	B	254	GLN
2	B	317	GLN
2	B	322	GLN
2	B	431	ASN
1	C	60	HIS
1	C	85	GLN
1	C	246	GLN
1	C	265	GLN
1	C	268	HIS
1	C	272	ASN
2	D	233	HIS
2	D	313	GLN
2	D	317	GLN
2	D	321	HIS
2	D	370	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	TPO	A	160	1	8,10,11	1.22	0	10,14,16	1.23	1 (10%)
1	TPO	C	160	1	8,10,11	1.94	2 (25%)	10,14,16	1.45	2 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	160	1	-	1/9/11/13	-
1	TPO	C	160	1	-	1/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	P-OG1	4.22	1.66	1.59
1	C	160	TPO	P-O2P	2.11	1.62	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	TPO	O-C-CA	-3.57	115.59	124.77
1	C	160	TPO	O3P-P-O1P	3.00	122.50	110.83
1	C	160	TPO	P-OG1-CB	-2.53	116.44	123.33

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	160	TPO	O-C-CA-CB
1	C	160	TPO	C-CA-CB-CG2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	160	TPO	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	2A6	A	1298	-	26,27,27	2.87	9 (34%)	32,36,36	2.61	11 (34%)
3	2A6	C	1298	-	26,27,27	3.54	10 (38%)	32,36,36	3.05	7 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	2A6	A	1298	-	-	3/9/17/17	0/4/4/4
3	2A6	C	1298	-	-	2/9/17/17	0/4/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1298	2A6	C4-N9	-10.48	1.29	1.38
3	A	1298	2A6	C4-N9	-9.51	1.30	1.38
3	C	1298	2A6	C4-N3	6.95	1.44	1.34
3	C	1298	2A6	O6-C10	-6.90	1.22	1.44
3	A	1298	2A6	C4-N3	6.12	1.42	1.34
3	C	1298	2A6	C5-N7	4.54	1.45	1.37
3	C	1298	2A6	C8-N7	-4.34	1.25	1.35
3	A	1298	2A6	C2-N1	4.25	1.46	1.34
3	C	1298	2A6	C2-N1	4.16	1.46	1.34
3	C	1298	2A6	C6-N1	-3.89	1.26	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1298	2A6	C5-C4	-3.83	1.33	1.40
3	A	1298	2A6	C5-N7	3.60	1.44	1.37
3	A	1298	2A6	C8-N7	-3.44	1.27	1.35
3	A	1298	2A6	C5-C4	-3.34	1.34	1.40
3	A	1298	2A6	C2-N2	-2.96	1.30	1.36
3	C	1298	2A6	C2-N3	-2.65	1.27	1.34
3	A	1298	2A6	C2-N3	-2.64	1.27	1.34
3	C	1298	2A6	C2-N2	-2.59	1.31	1.36
3	A	1298	2A6	C17-N2	-2.38	1.35	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1298	2A6	N3-C4-N9	9.19	133.08	125.68
3	C	1298	2A6	C4-N9-C8	7.62	108.69	103.84
3	C	1298	2A6	C5-C4-N3	-7.05	118.01	124.22
3	C	1298	2A6	N3-C2-N1	-6.82	115.08	126.26
3	A	1298	2A6	C4-C5-N7	-6.59	100.85	105.28
3	A	1298	2A6	C5-C4-N3	-5.06	119.76	124.22
3	A	1298	2A6	N3-C2-N1	-5.01	118.05	126.26
3	A	1298	2A6	C2-N1-C6	4.36	122.89	115.38
3	C	1298	2A6	C2-N1-C6	4.33	122.84	115.38
3	A	1298	2A6	C4-N9-C8	3.75	106.22	103.84
3	A	1298	2A6	O6-C6-C5	3.71	121.74	115.40
3	A	1298	2A6	N2-C2-N1	3.68	129.55	116.90
3	A	1298	2A6	C17-N2-C2	-3.56	119.79	129.38
3	A	1298	2A6	C5-C4-N9	3.31	113.10	110.46
3	C	1298	2A6	N2-C2-N3	2.55	125.67	116.90
3	A	1298	2A6	C5-N7-C8	2.48	108.34	106.27
3	A	1298	2A6	C14-C13-C12	2.07	115.68	111.42
3	C	1298	2A6	C14-C13-C12	2.06	115.64	111.42

There are no chirality outliers.

All (5) torsion outliers are listed below:

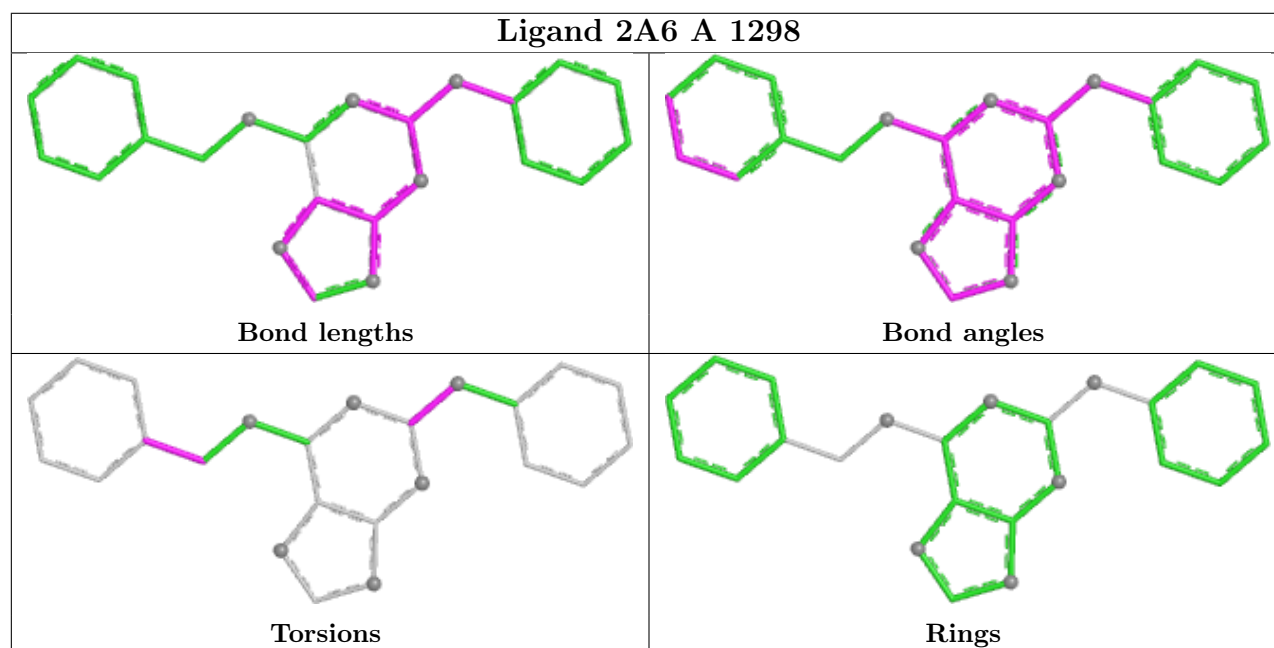
Mol	Chain	Res	Type	Atoms
3	A	1298	2A6	O6-C10-C11-C12
3	A	1298	2A6	O6-C10-C11-C16
3	C	1298	2A6	O6-C10-C11-C16
3	A	1298	2A6	N3-C2-N2-C17
3	C	1298	2A6	O6-C10-C11-C12

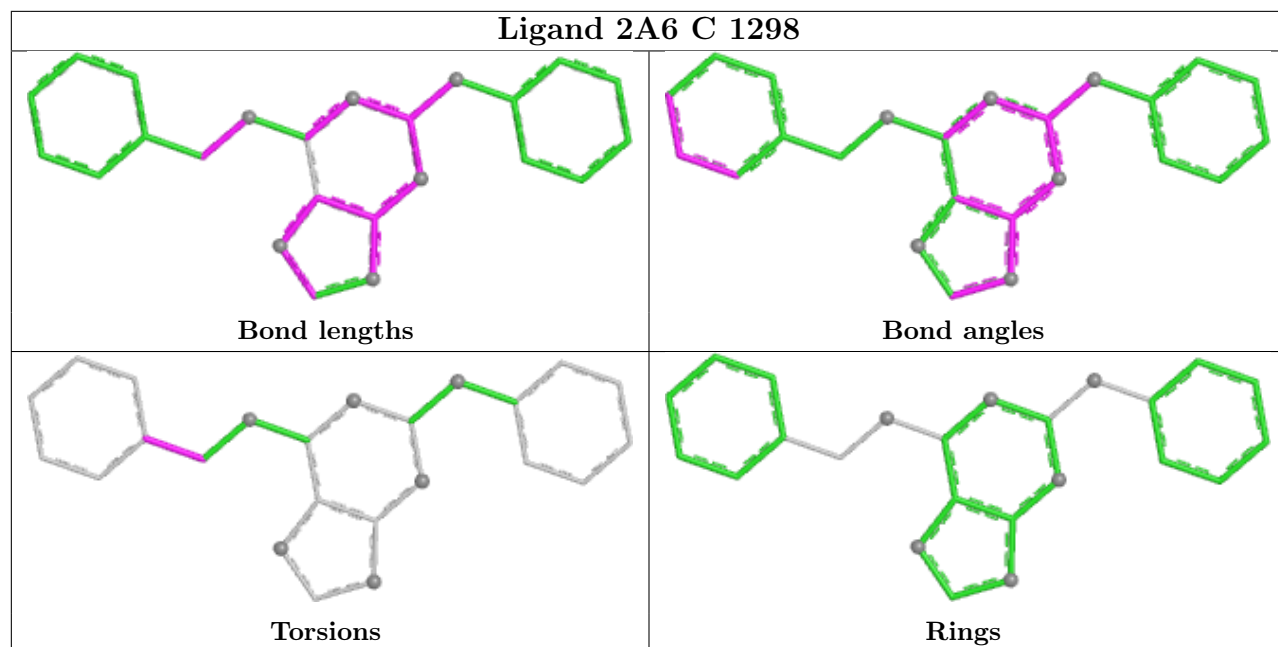
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1298	2A6	2	0
3	C	1298	2A6	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	296/303 (97%)	0.40	37 (12%) 8 6	25, 43, 121, 177	0
1	C	296/303 (97%)	1.06	51 (17%) 4 3	36, 61, 119, 178	0
2	B	258/258 (100%)	-0.02	9 (3%) 47 42	24, 40, 75, 143	0
2	D	258/258 (100%)	0.68	24 (9%) 14 12	32, 58, 87, 148	0
All	All	1108/1122 (98%)	0.54	121 (10%) 10 9	24, 52, 105, 178	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	40	GLU	7.2
1	C	39	THR	7.2
1	A	294	PRO	7.1
1	A	296	LEU	7.0
1	A	96	LEU	6.5
2	D	175	VAL	6.2
1	C	38	ASP	6.2
2	B	432	LEU	5.6
1	C	296	LEU	5.6
1	A	95	ALA	5.5
2	B	175	VAL	5.5
1	C	37	LEU	5.4
1	A	97	THR	5.3
1	A	293	VAL	5.1
1	C	96	LEU	5.1
1	A	295	HIS	5.0
1	A	248	PHE	4.9
1	A	72	THR	4.8
1	C	72	THR	4.6
1	C	41	THR	4.6
1	C	97	THR	4.5

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Mol	Chain	Res	Type	RSRZ
2	D	432	LEU	4.5
1	A	37	LEU	4.3
1	C	93	ALA	4.2
1	A	38	ASP	4.1
1	A	71	HIS	4.1
1	A	39	THR	3.9
1	C	71	HIS	3.9
1	C	74	ASN	3.8
1	A	36	ARG	3.8
2	B	177	ASP	3.8
1	C	98	GLY	3.8
1	A	99	ILE	3.8
2	D	430	LEU	3.7
1	C	73	GLU	3.7
2	D	372	TRP	3.7
1	C	294	PRO	3.7
1	C	99	ILE	3.6
1	C	35	ILE	3.6
1	C	100	PRO	3.5
1	C	293	VAL	3.5
2	B	176	PRO	3.5
1	A	41	THR	3.4
1	A	35	ILE	3.4
1	C	227	TRP	3.3
1	A	98	GLY	3.3
2	B	430	LEU	3.3
1	C	213	PHE	3.3
1	C	161	HIS	3.3
1	A	40	GLU	3.2
1	C	95	ALA	3.1
2	B	429	THR	3.1
1	C	295	HIS	3.0
1	A	200	ARG	3.0
1	A	250	LYS	3.0
1	A	246	GLN	2.9
1	C	225	VAL	2.9
1	C	36	ARG	2.8
1	C	289	VAL	2.8
1	C	101	LEU	2.8
1	C	238	PRO	2.8
1	C	231	THR	2.8
1	A	247	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	382	TYR	2.8
1	A	74	ASN	2.8
2	B	428	GLU	2.8
1	A	292	PRO	2.7
1	C	251	VAL	2.7
1	C	233	MET	2.7
1	A	179	TYR	2.7
2	D	176	PRO	2.6
2	D	431	ASN	2.6
1	C	94	SER	2.6
1	A	100	PRO	2.6
1	C	292	PRO	2.6
1	A	94	SER	2.6
2	D	324	PRO	2.5
1	C	223	ASP	2.5
2	D	323	GLN	2.5
1	A	249	SER	2.5
2	D	429	THR	2.5
2	D	426	PRO	2.5
1	A	199	ARG	2.5
1	A	101	LEU	2.4
1	A	75	LYS	2.4
1	C	70	ILE	2.4
1	A	161	HIS	2.4
2	D	418	TYR	2.4
1	C	248	PHE	2.3
1	C	162	GLU	2.3
2	B	385	GLU	2.3
2	D	358	ALA	2.3
1	C	246	GLN	2.3
1	C	42	GLU	2.3
1	C	226	VAL	2.3
2	D	402	PRO	2.3
1	C	199	ARG	2.3
1	A	73	GLU	2.3
2	D	369	GLY	2.2
1	C	163	VAL	2.2
1	A	15	TYR	2.2
1	C	216	PHE	2.2
2	B	431	ASN	2.2
2	D	327	CYS	2.2
2	D	399	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	0	SER	2.2
1	C	131	GLN	2.1
2	D	384	LEU	2.1
2	D	177	ASP	2.1
1	C	285	PHE	2.1
1	A	93	ALA	2.1
1	C	179	TYR	2.1
2	D	335	PHE	2.1
2	D	362	LEU	2.1
2	D	329	VAL	2.0
2	D	334	MET	2.0
2	D	390	CYS	2.0
1	C	2	GLU	2.0
1	C	237	LYS	2.0
1	A	70	ILE	2.0
1	C	243	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPO	C	160	11/12	0.92	0.21	20,20,20,20	0
1	TPO	A	160	11/12	0.97	0.07	38,40,52,53	0

6.3 Carbohydrates [i](#)

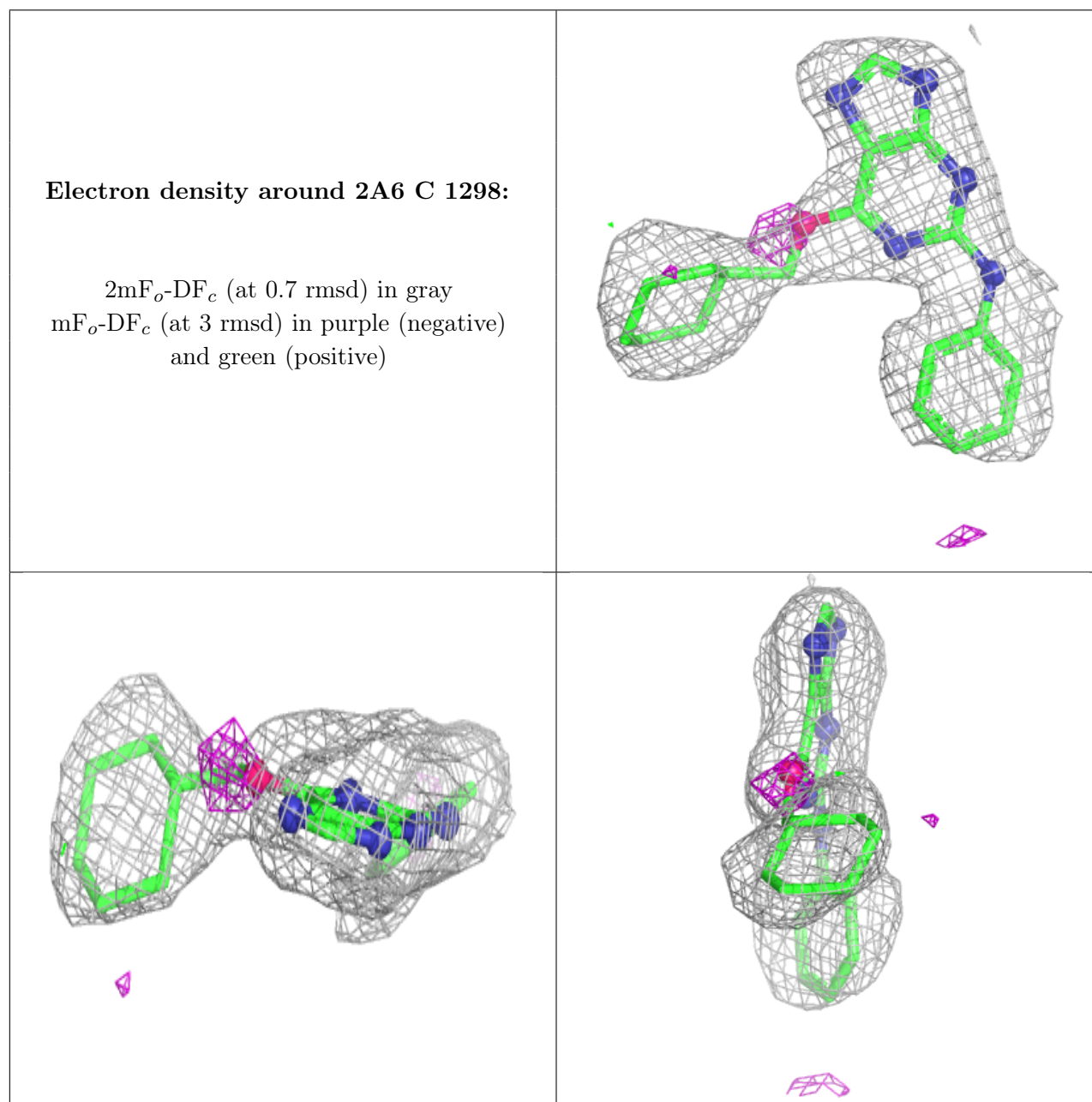
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

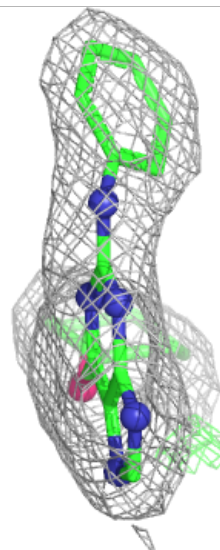
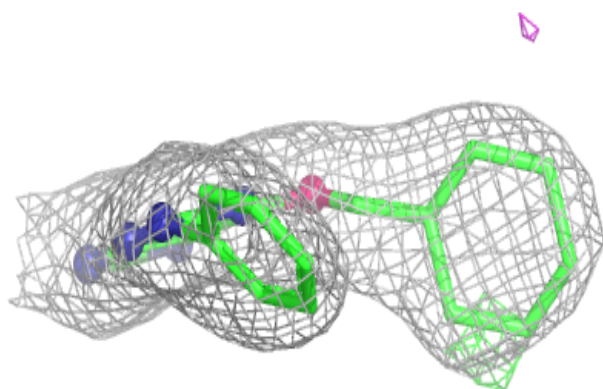
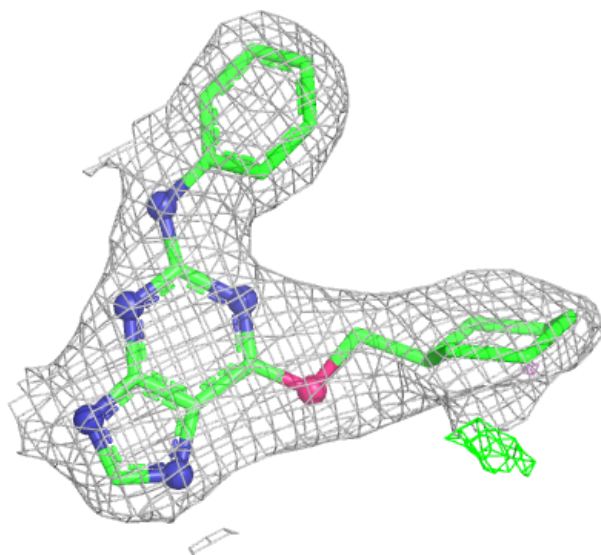
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	2A6	C	1298	24/24	0.86	0.12	47,51,54,55	0
3	2A6	A	1298	24/24	0.93	0.09	53,54,55,55	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around 2A6 A 1298:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.